

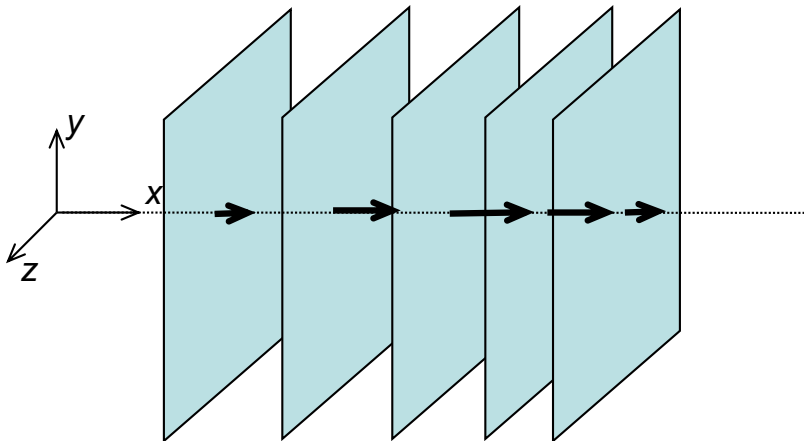
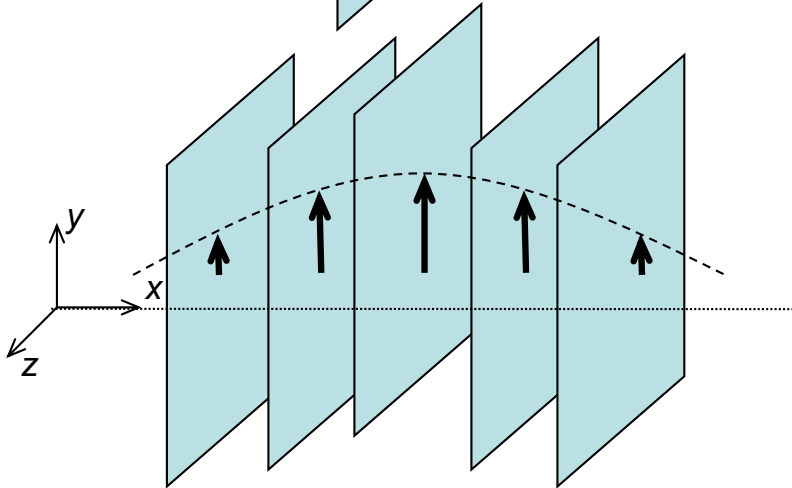
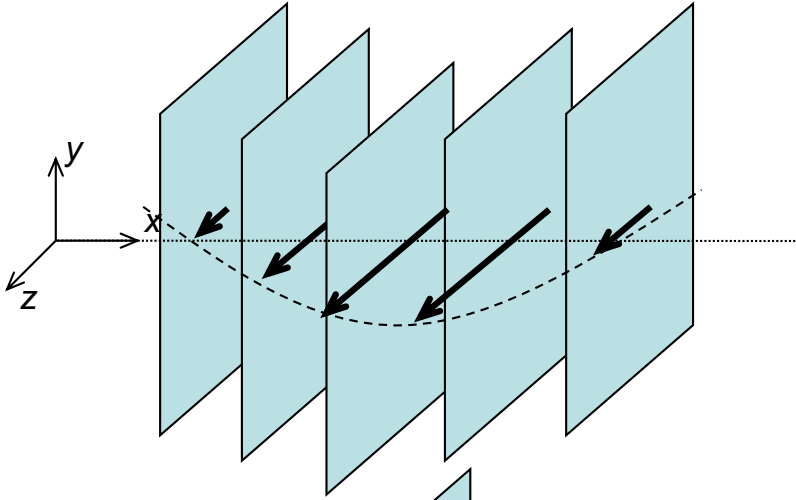


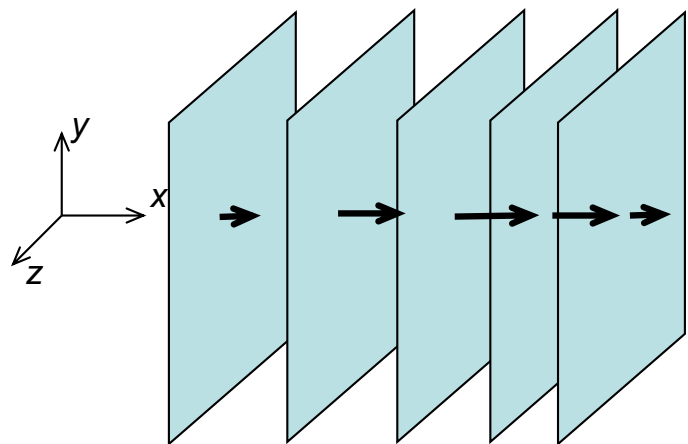
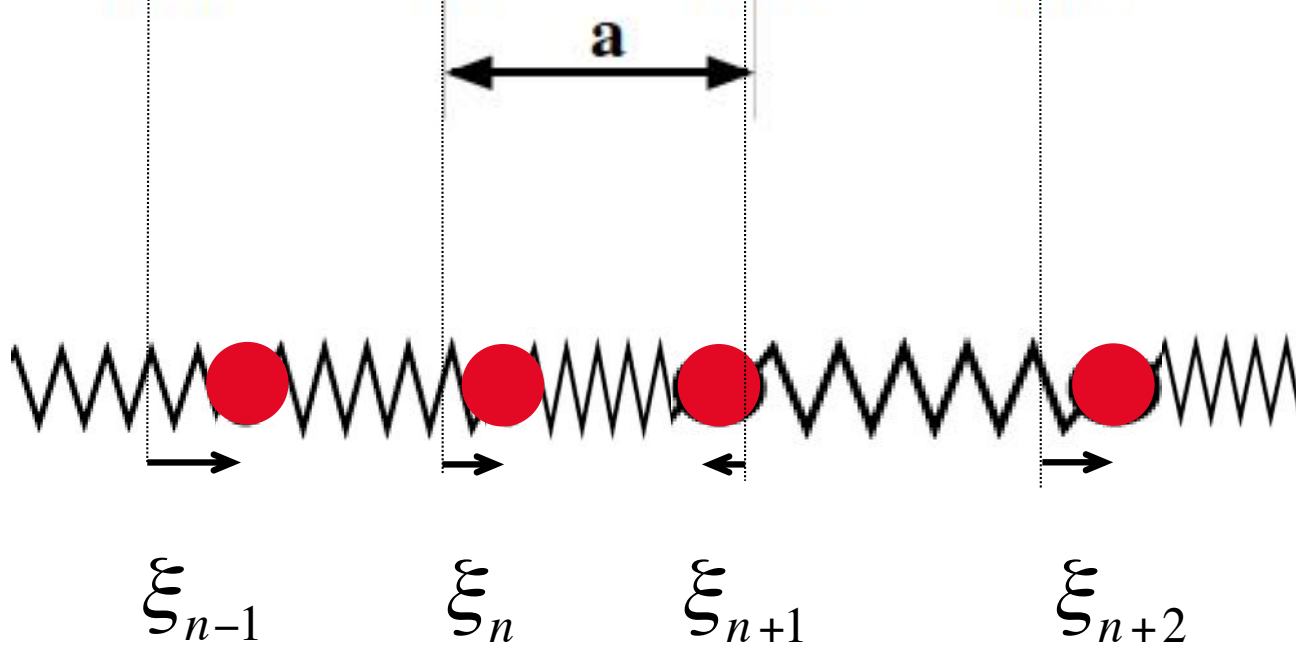
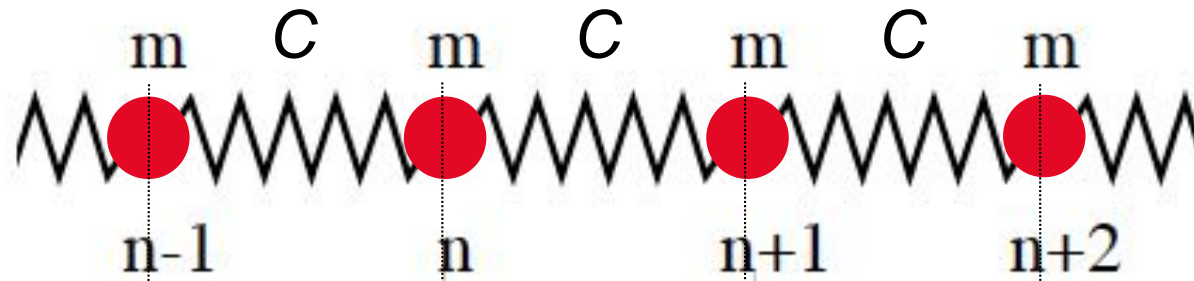
## IV. Phononen

Für jeden Wellenvektor  $\vec{k}$   
senkrecht zu Netzebenen  $(h k l)$   
3 Schwingungszustände:

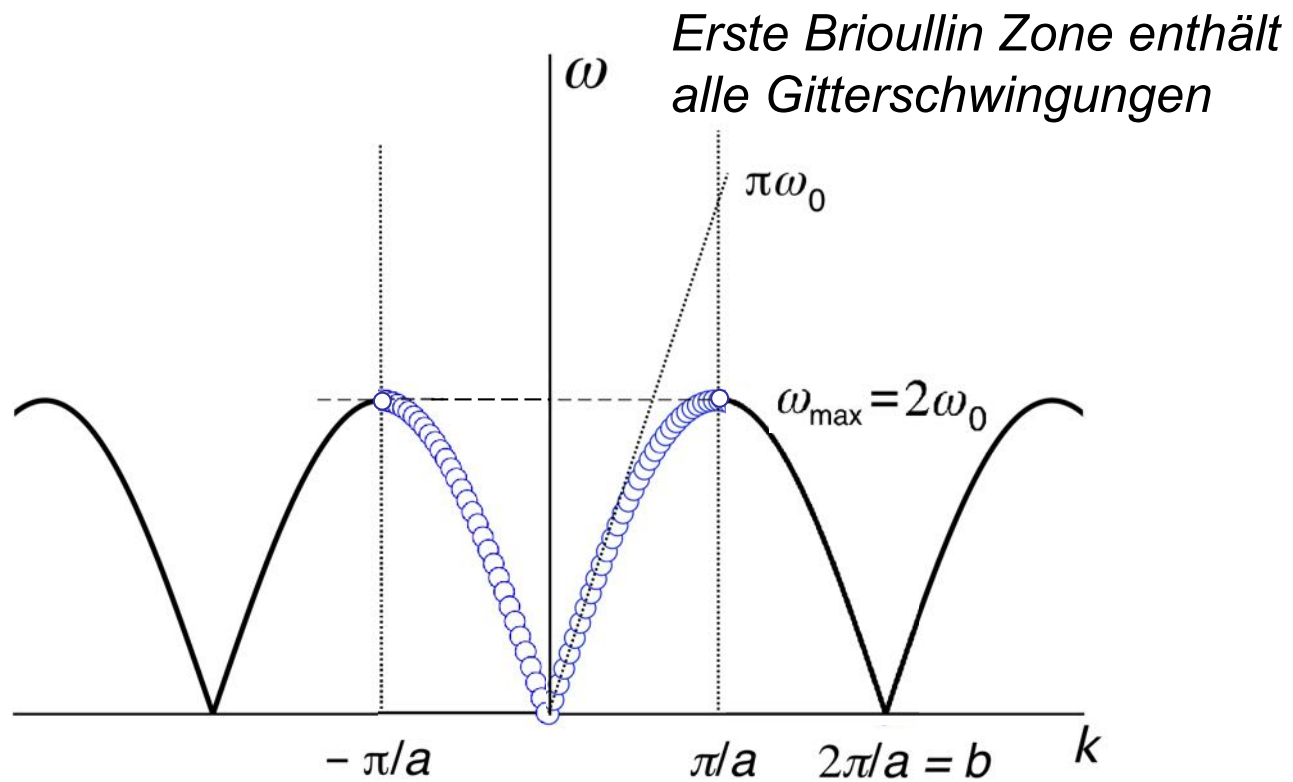
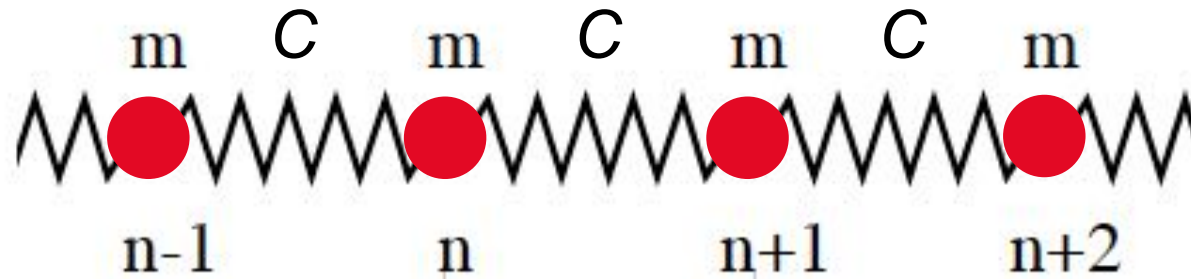
2 x transversal

1 x longitudinal

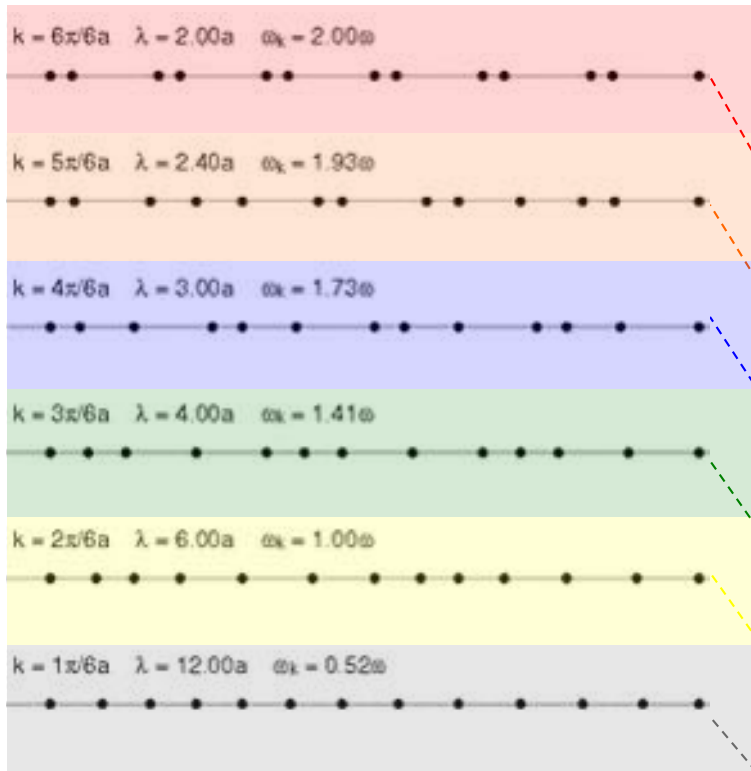




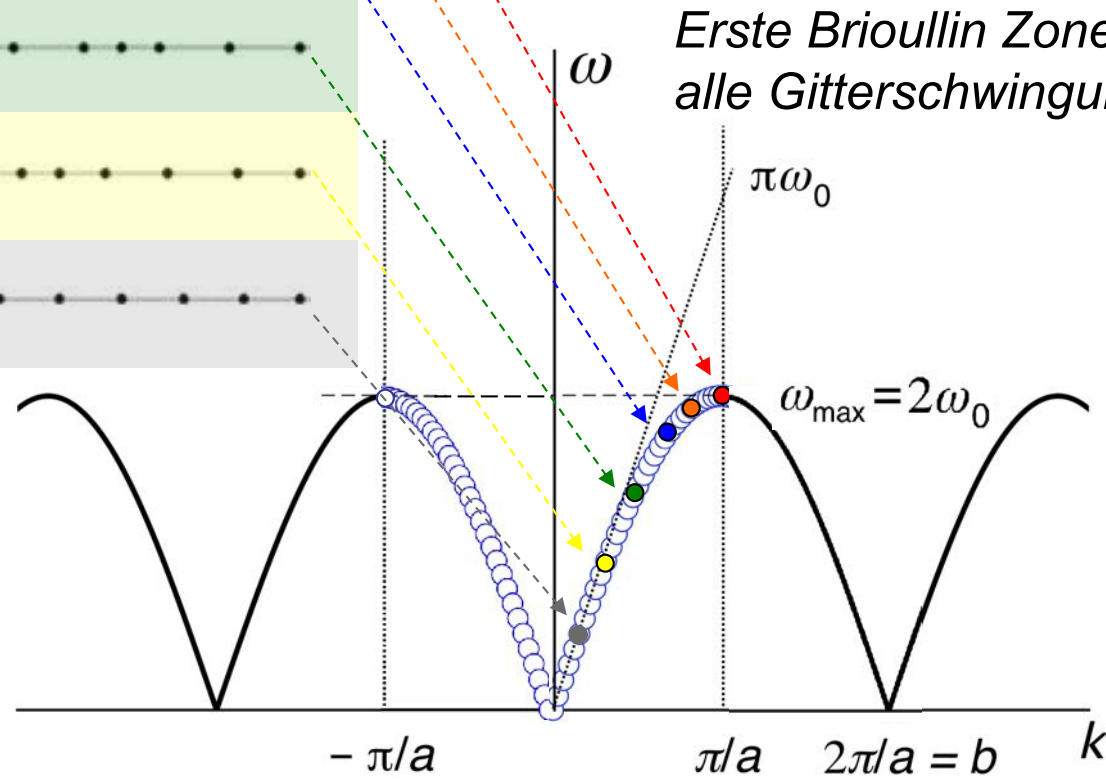
Modell: lineare Federkette



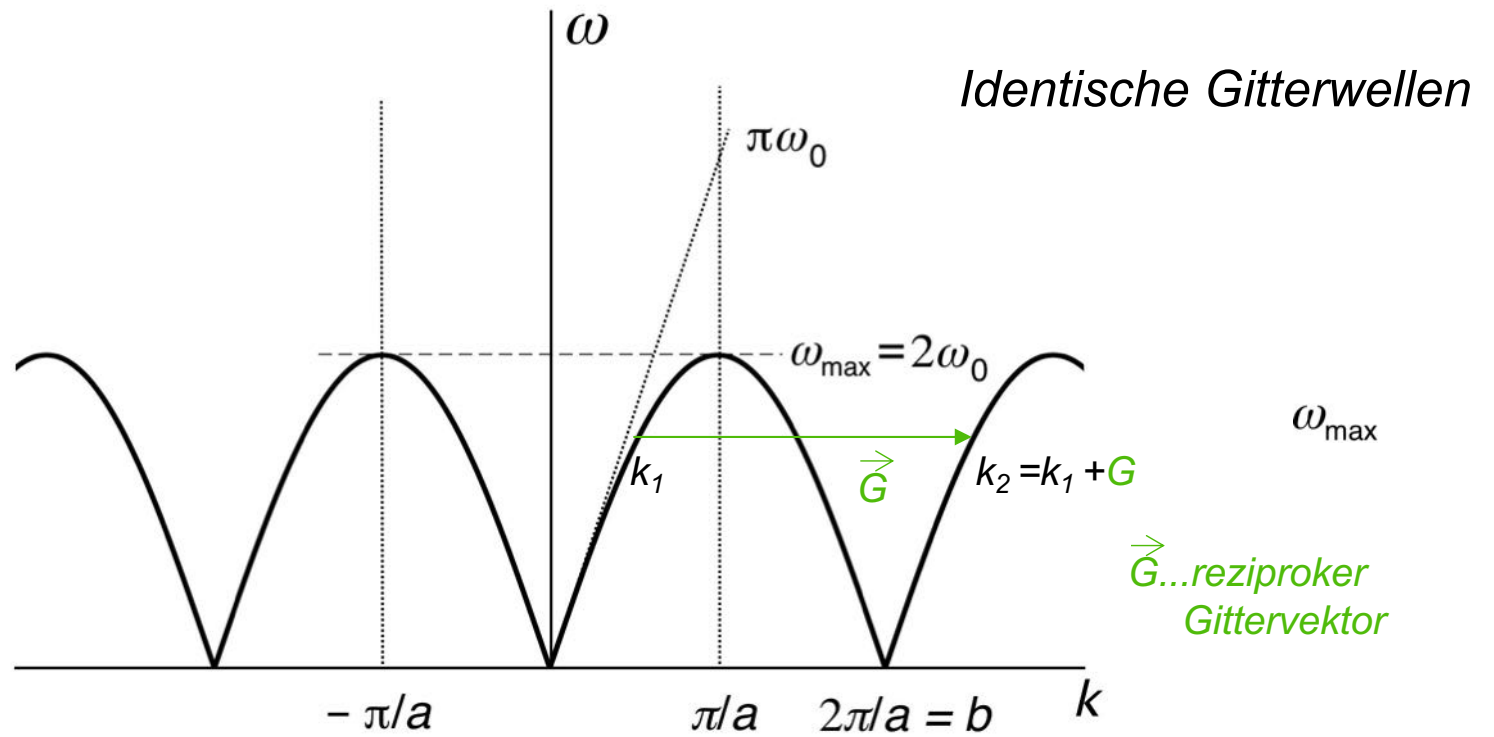
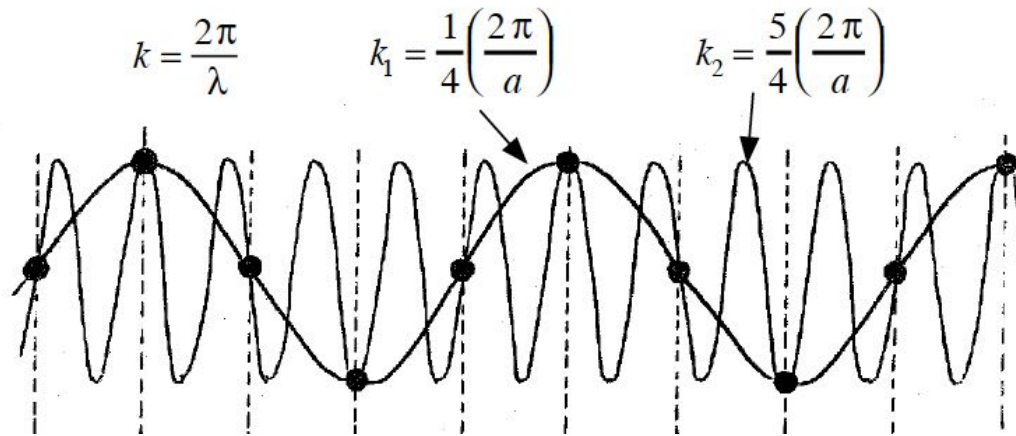
$N$  Atome mit periodischen Randbedingungen



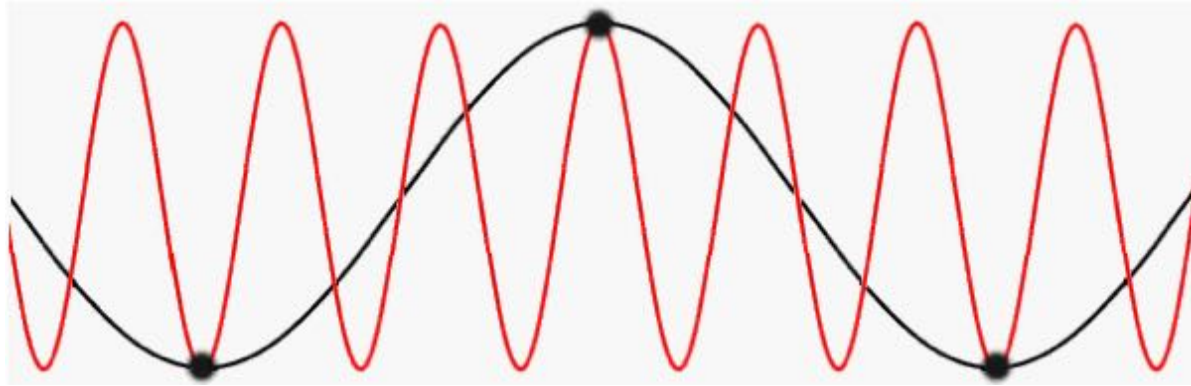
$\omega_{\max}$  : stehende Welle; Gruppengeschwindigkeit  $d\omega/dk = 0$



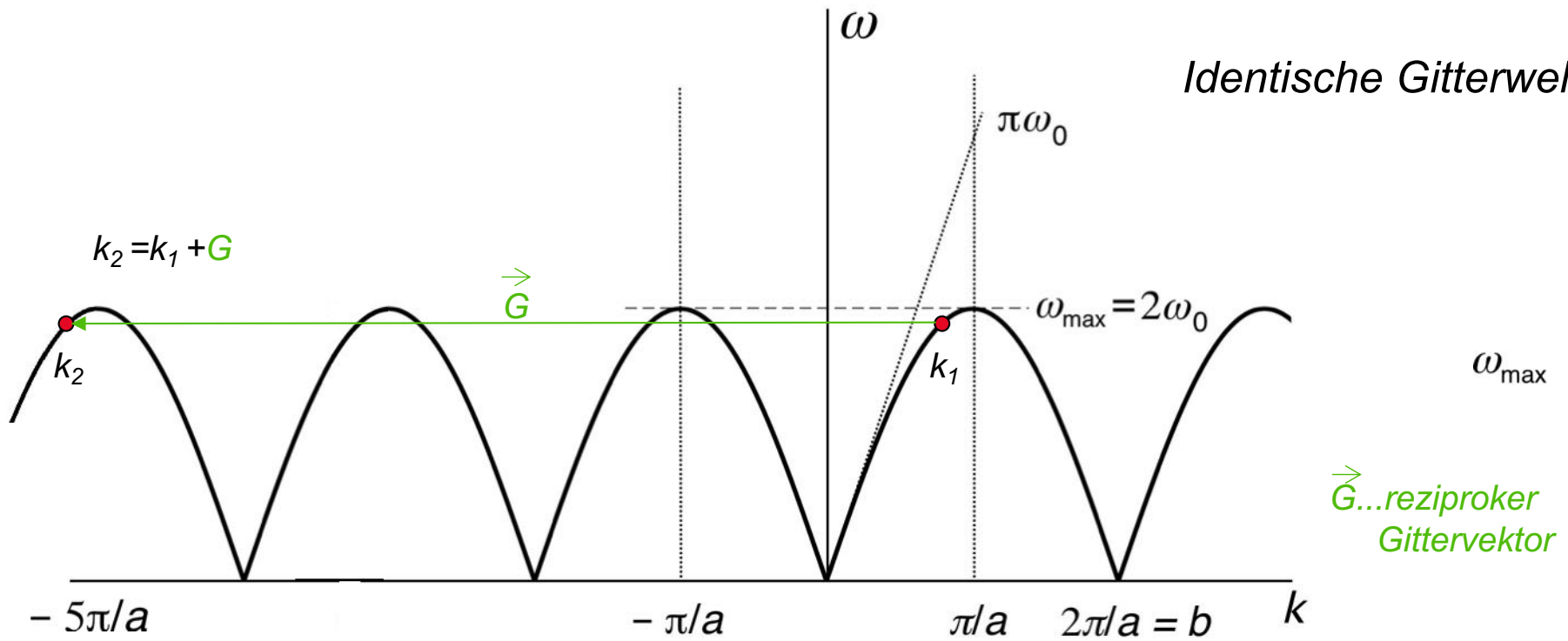
$N$  Atome mit periodischen Randbedingungen

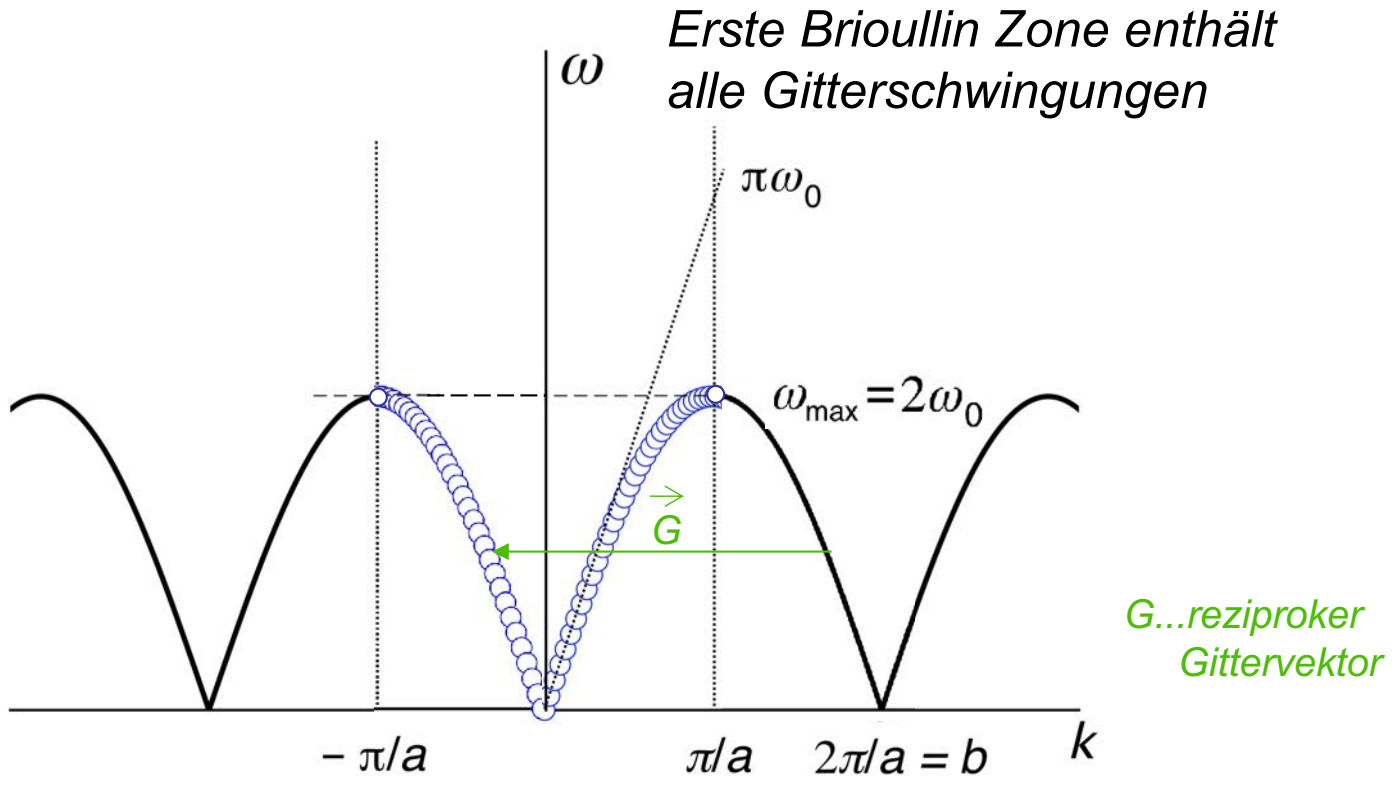
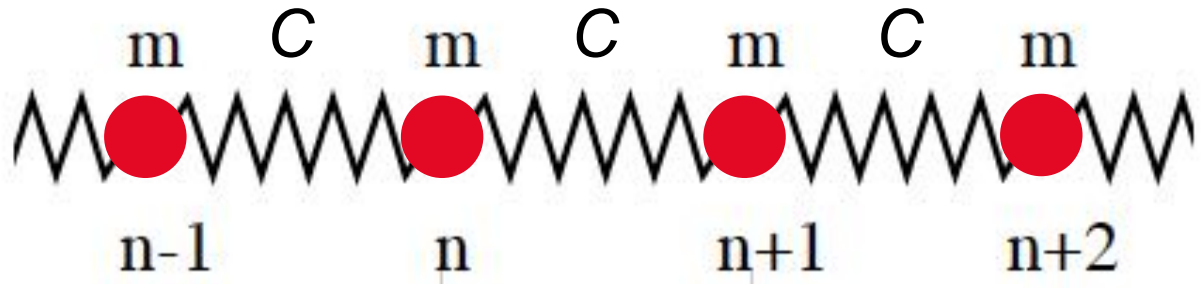






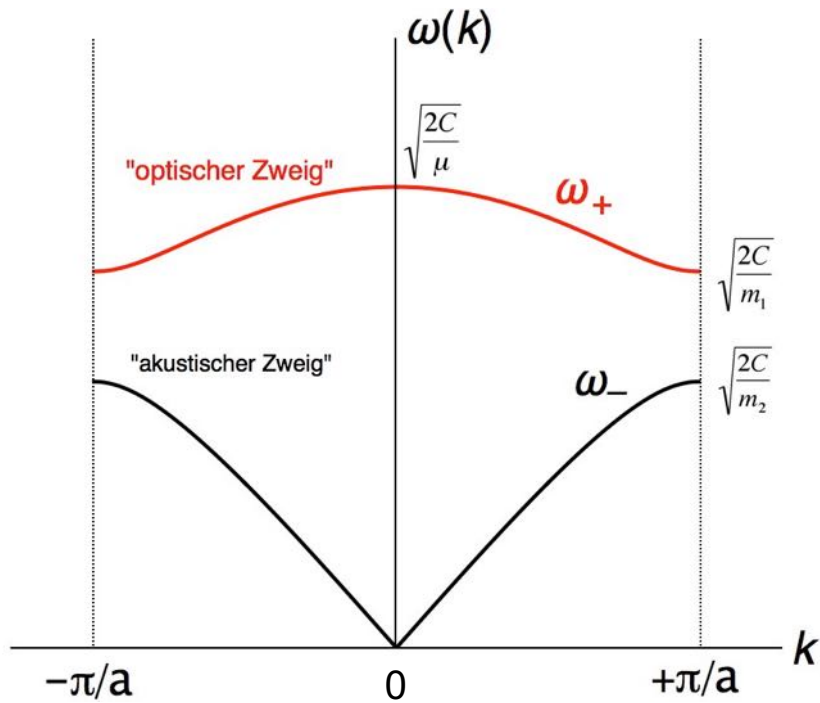
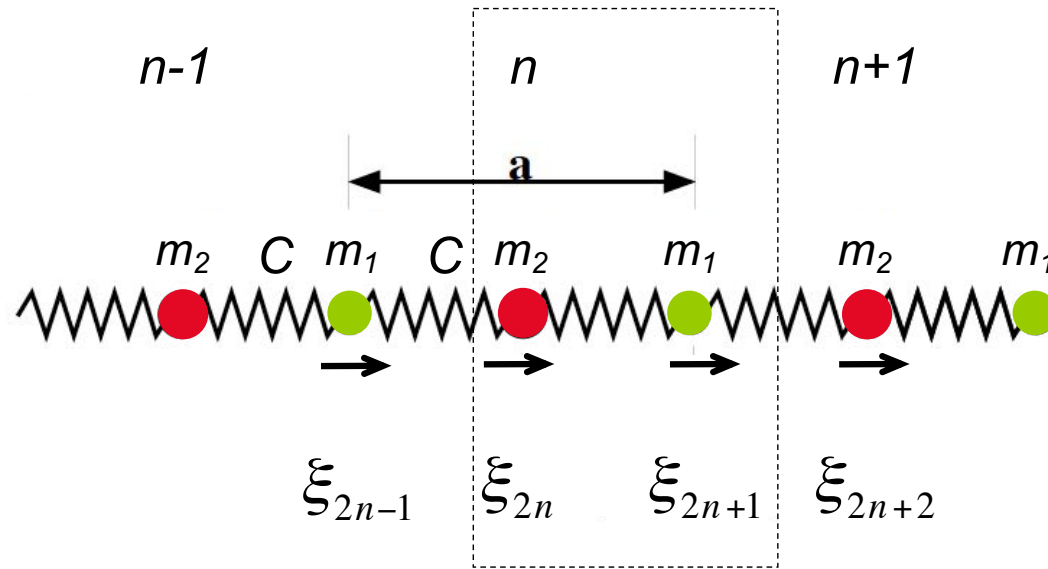
Identische Gitterwellen



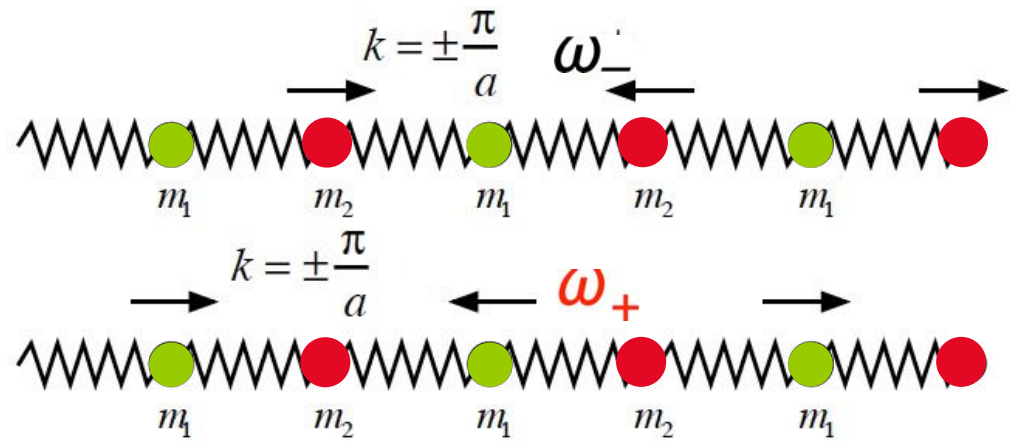
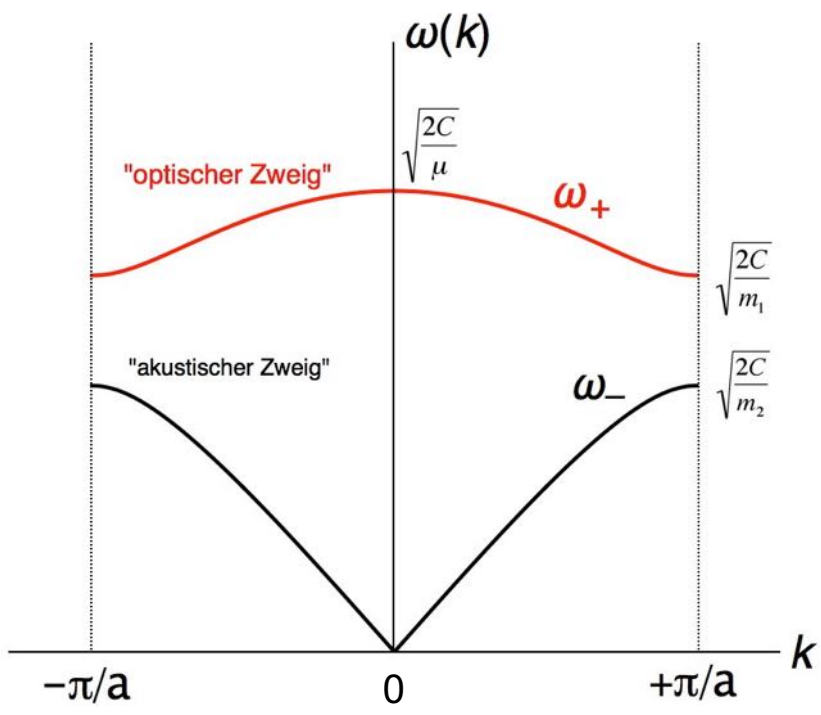
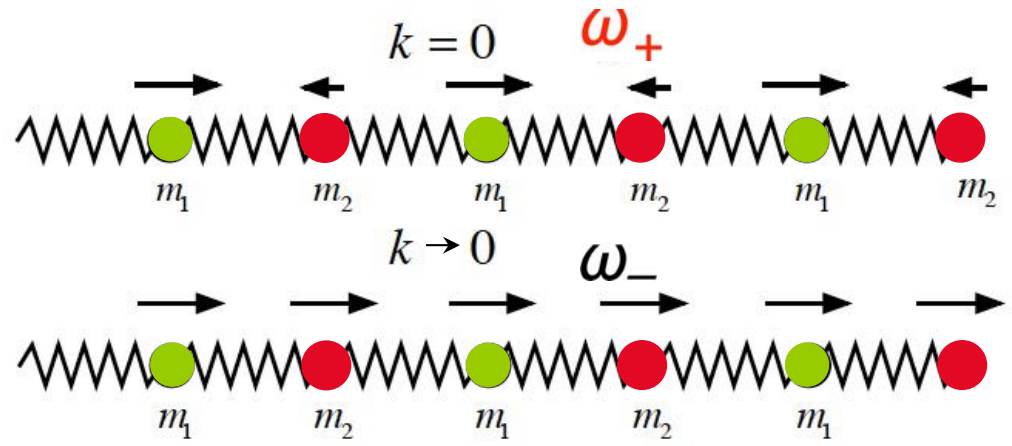


$N$  Atome mit periodischen Randbedingungen

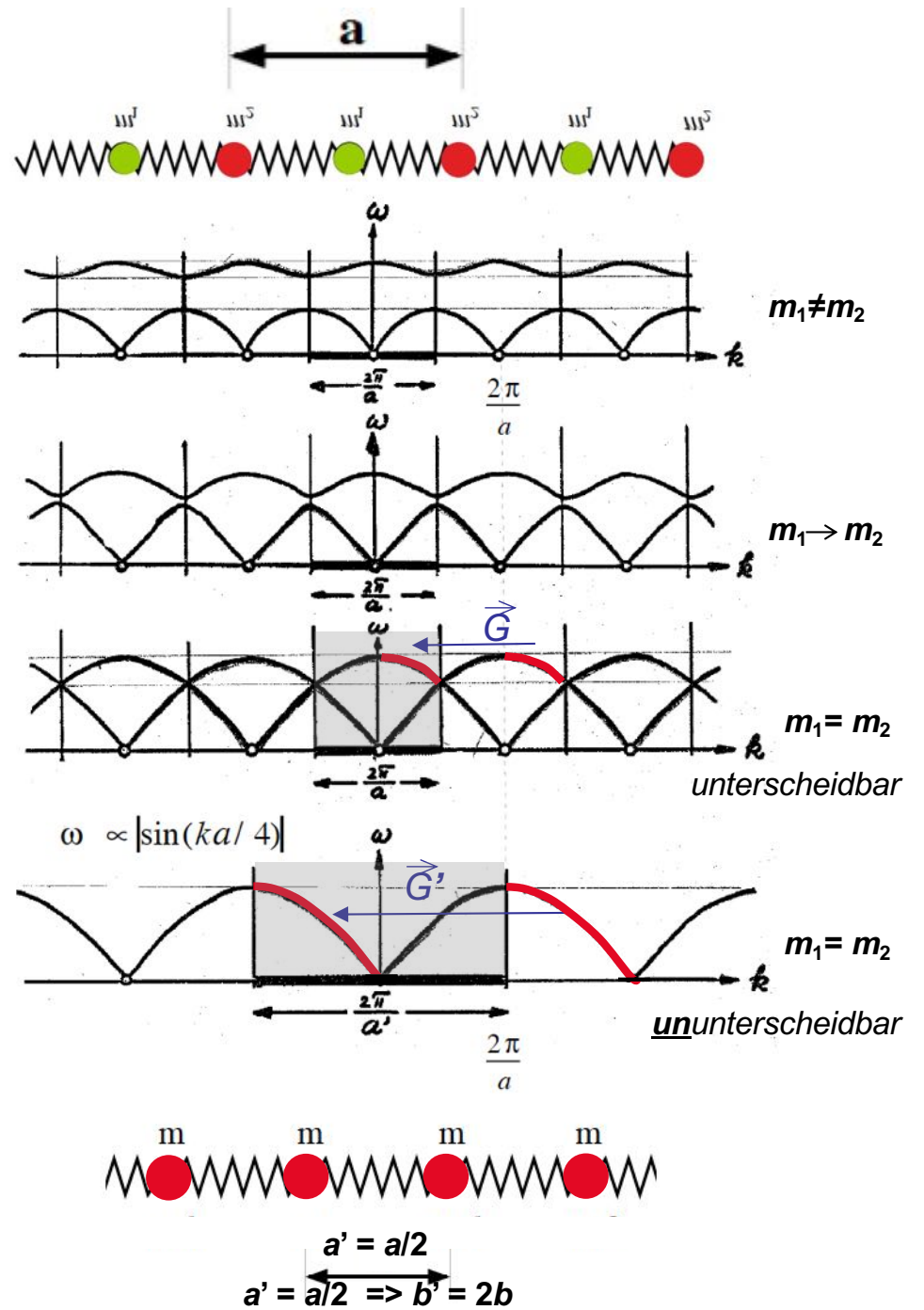
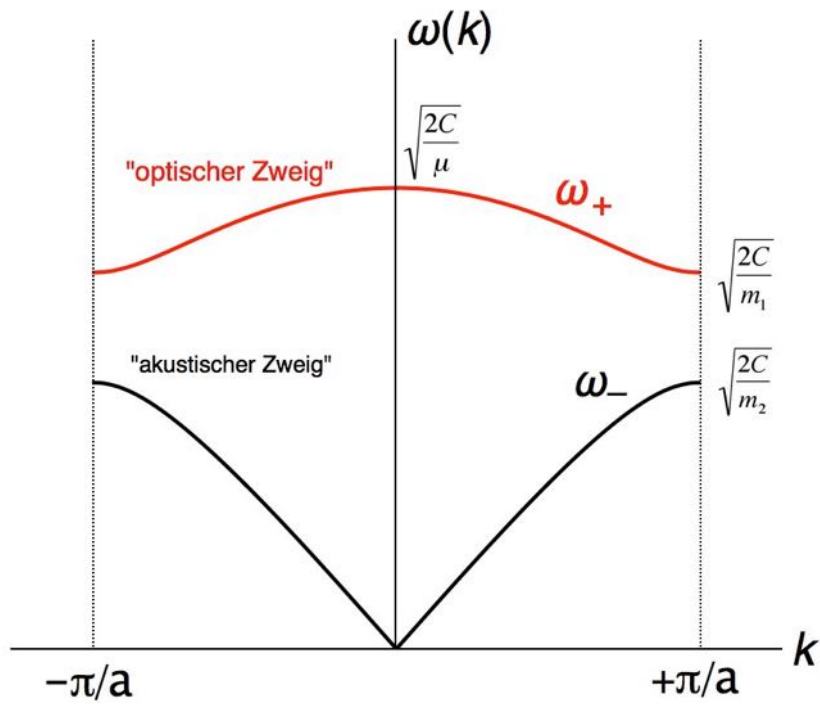




lineare Federkette mit 2-atomiger Basis



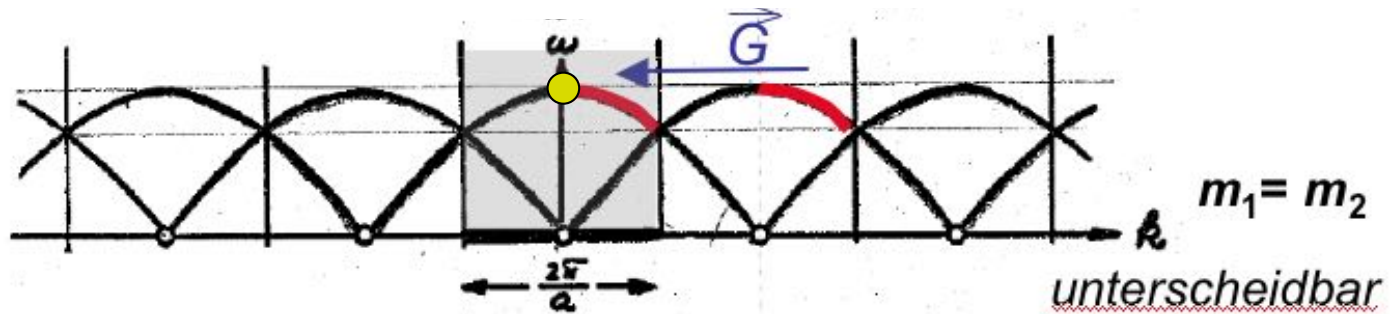
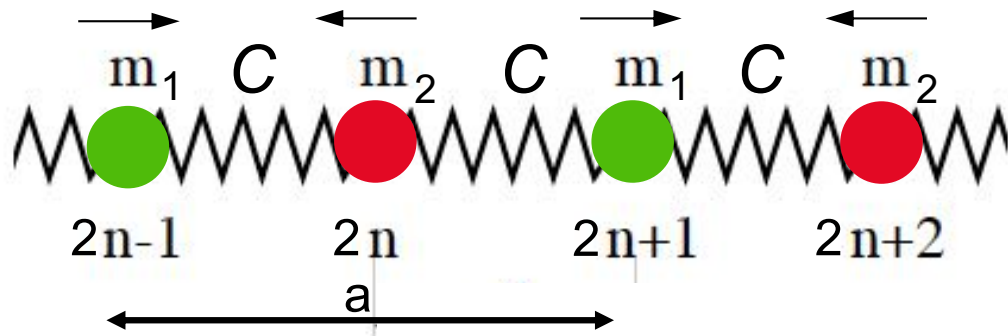
lineare Federkette mit 2-atomiger Basis



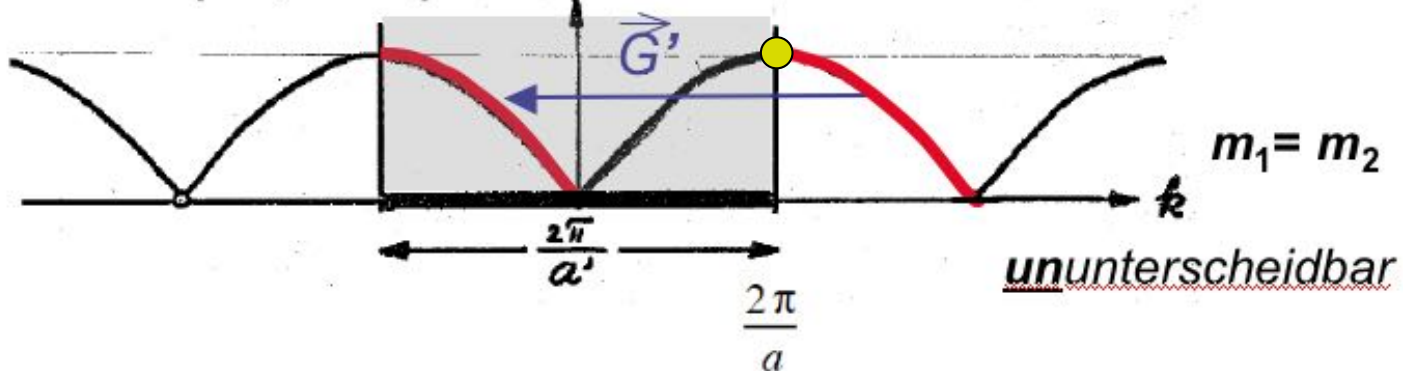
lineare Federkette mit 2-atomiger Basis

$$\lambda = \infty$$

$$k = 0$$

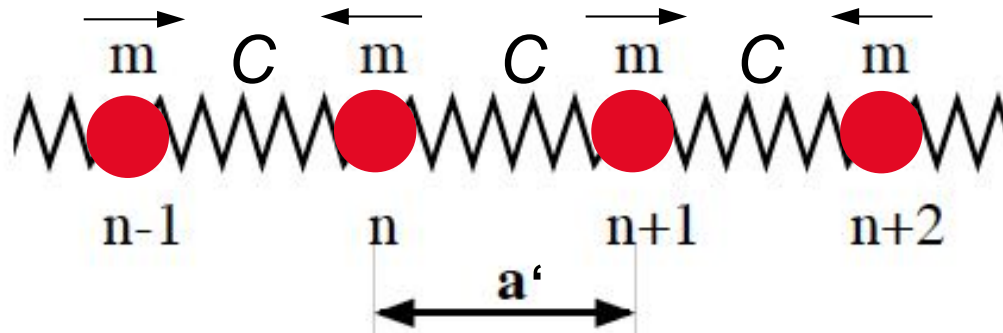


$$\omega \propto |\sin(ka/4)|$$



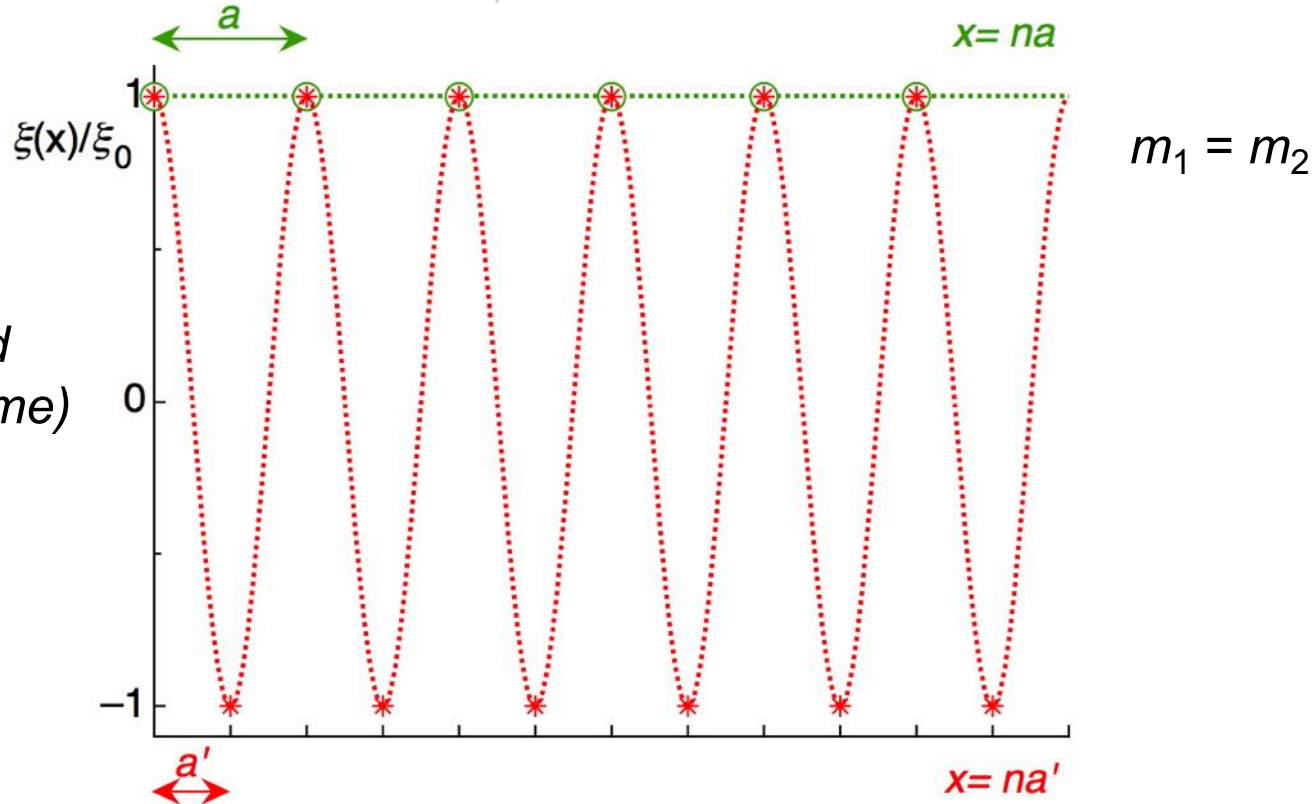
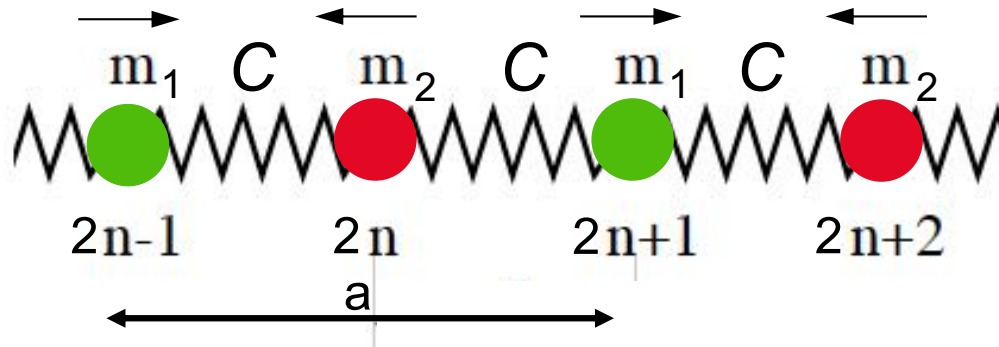
$$\lambda = 2a'$$

$$k = 2\pi / \lambda = \pi / a'$$



$$\lambda = \infty$$

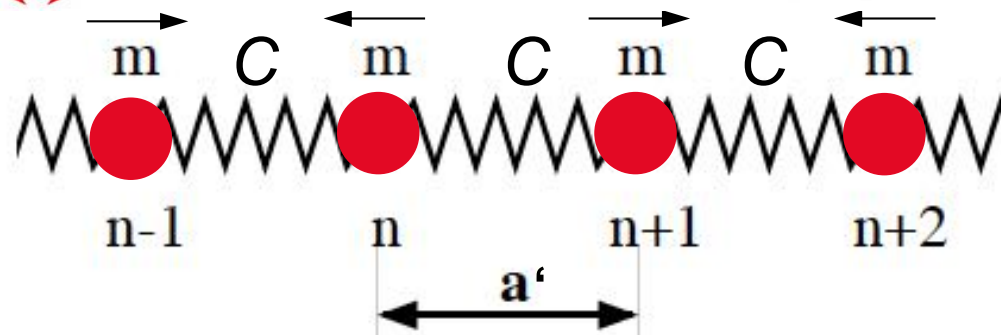
$$k = 0$$



Schwingungsbild  
(Momentaufnahme)

$$\lambda = 2a'$$

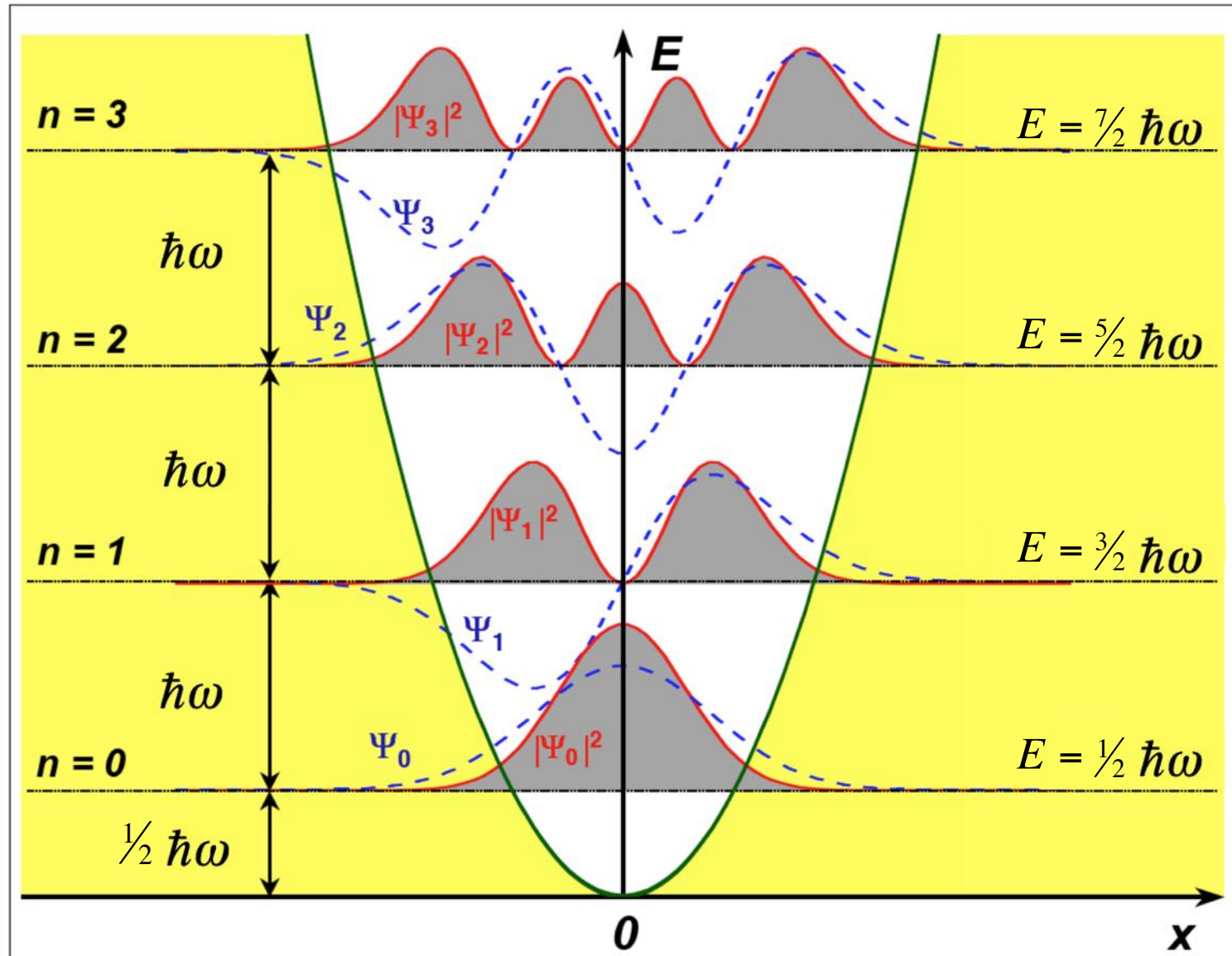
$$k = 2\pi / \lambda = \pi / a'$$





Erzeugung  
von Phononen  
durch  
Energiezufuhr

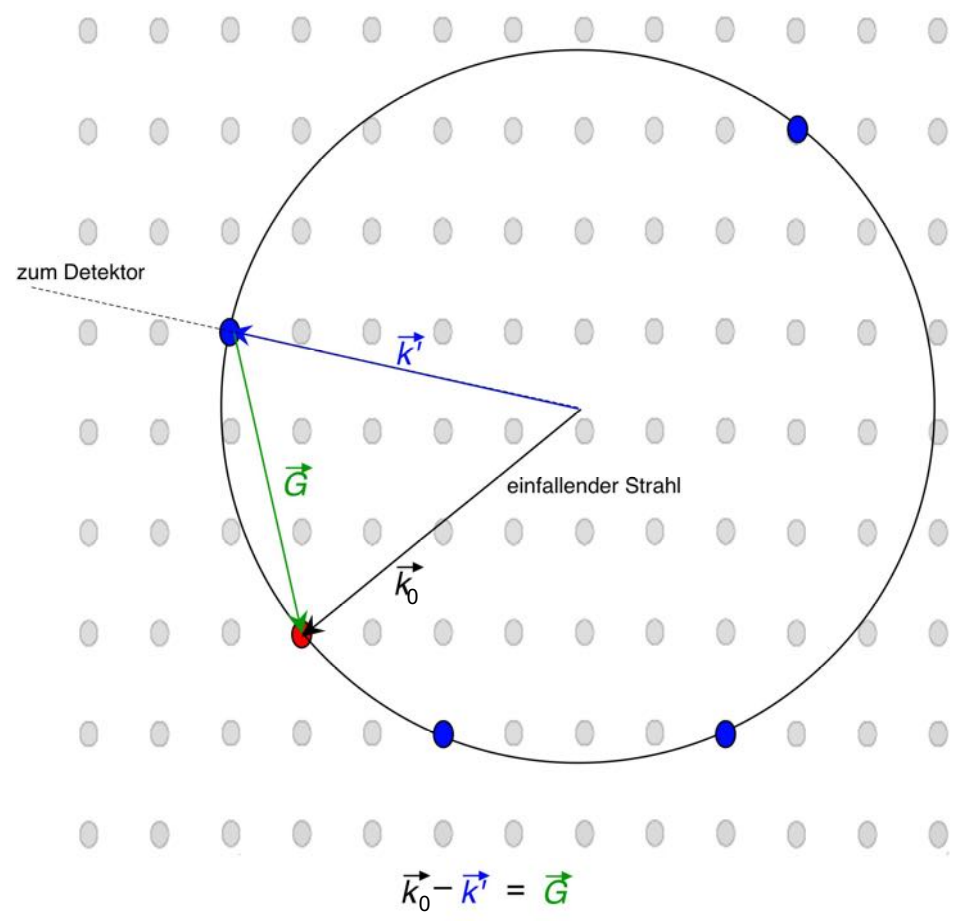
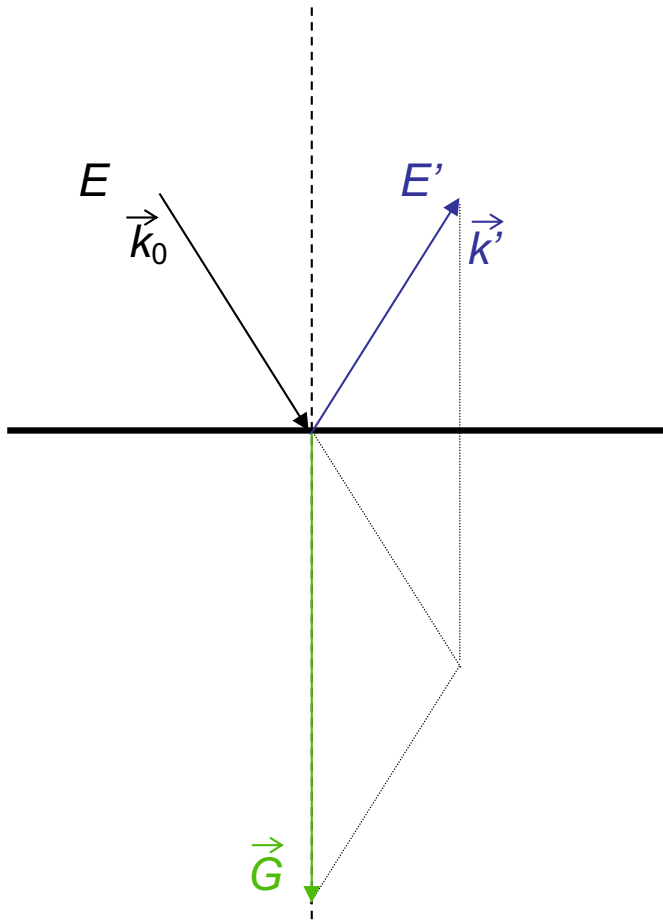
1D- quantenmechanischer harmonischer Oszillator mit  $\omega$



Vernichtung von  
Phononen  
durch  
Energieabgabe



# Elastische Streuung von Licht/Neutronen:

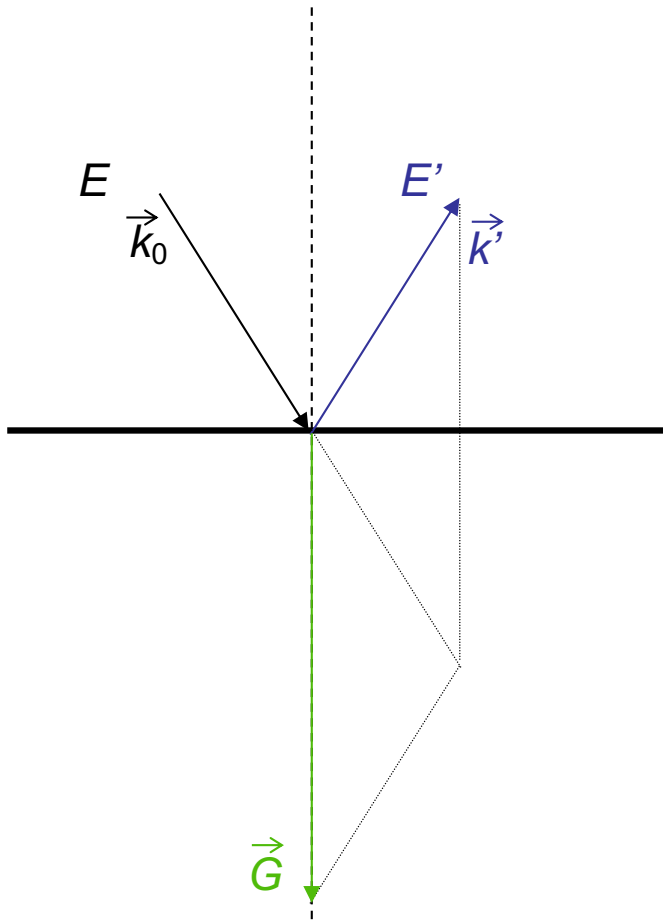


$$\vec{k}_0 - \vec{k}' = \vec{G} \quad (\text{Reziproker Gittervektor})$$

$$E - E' = 0$$

$\vec{k}'$  auf der Ewald-Kugel;  
keine Erzeugung von Phononen!

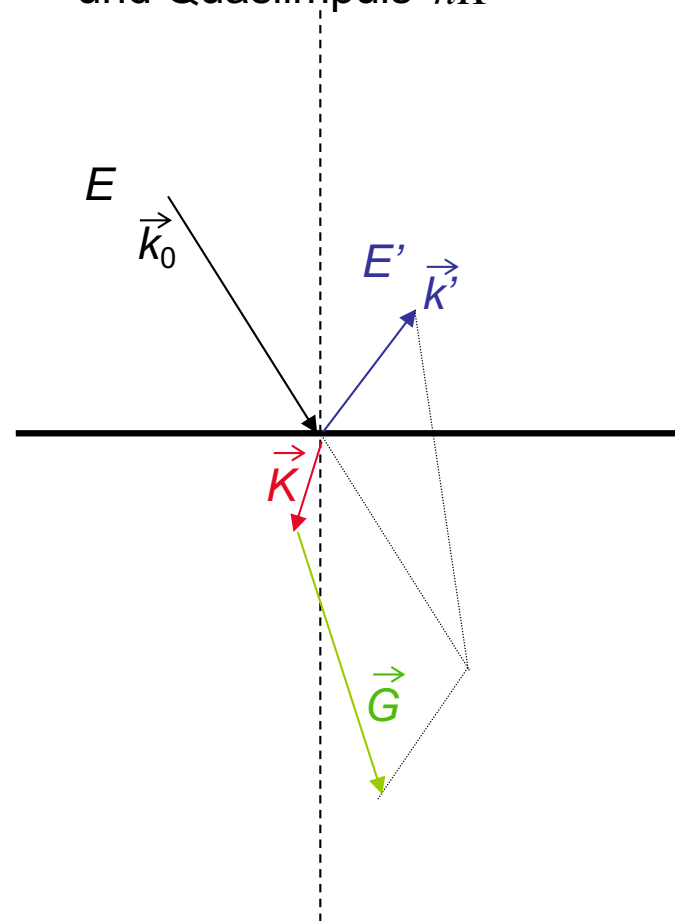
Elastische Streuung von Licht/Neutronen:



$$\vec{k}_0 - \vec{k}' = \vec{G} \quad (\text{Reziproker Gittervektor})$$

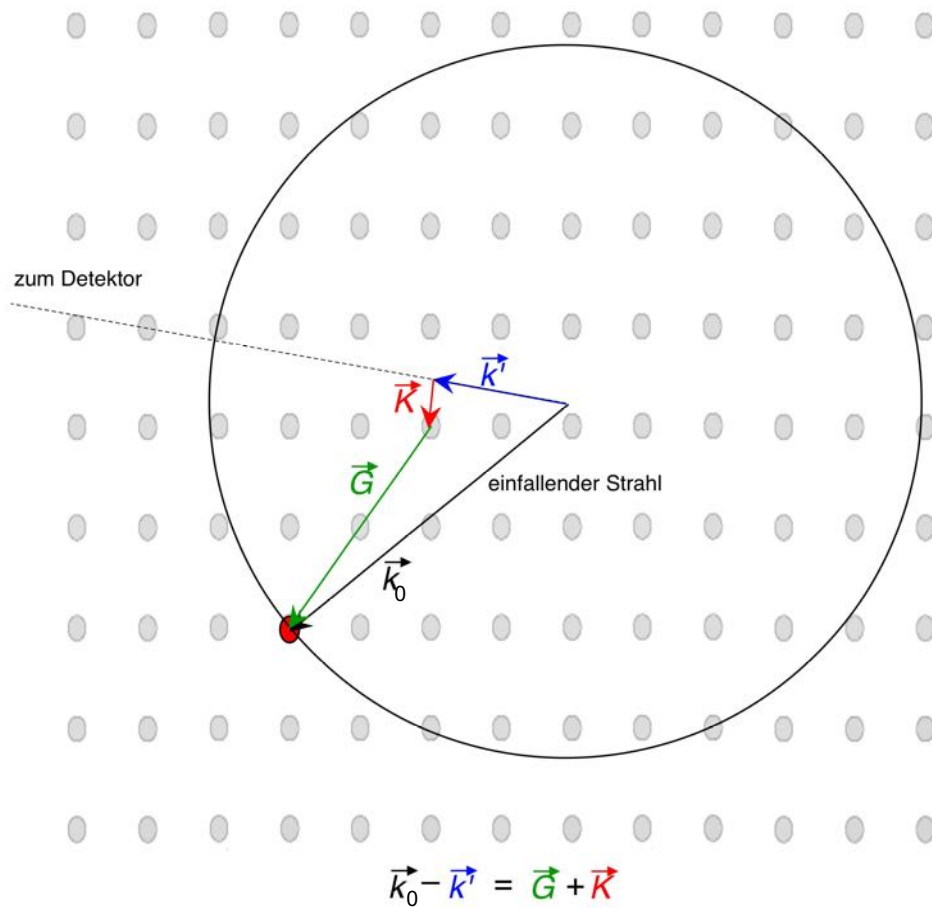
$$E - E' = 0$$

Inelastische Streuung:  
Erzeugung eines Phonons  
mit Energie  $\hbar\omega(\vec{K})$   
und Quasiimpuls  $\hbar\vec{K}$

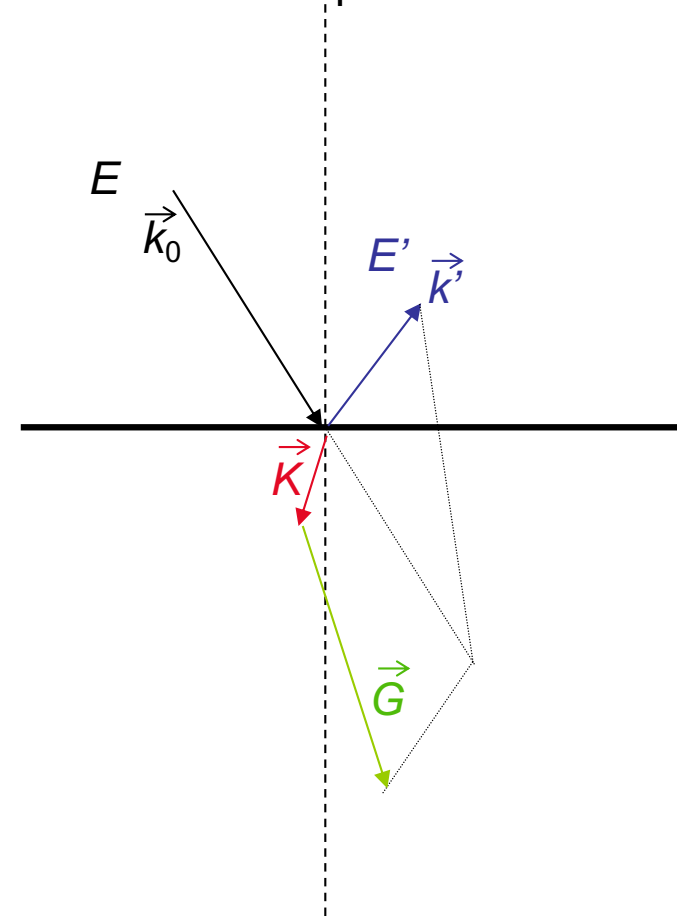


$$\vec{k}_0 - \vec{k}' = \vec{K} + \vec{G}$$

$$|E - E'| = \hbar\omega(\vec{K})$$



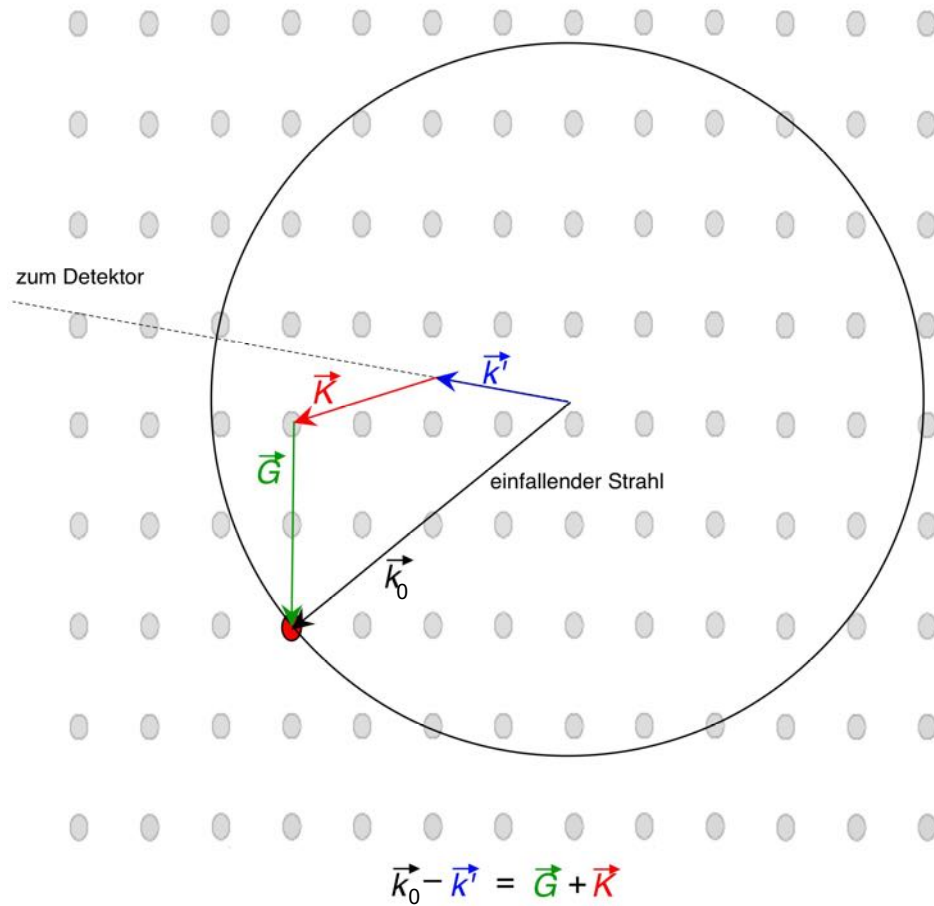
Inelastische Streuung:  
Erzeugung eines Phonons  
mit Energie  $\hbar\omega(\vec{K})$   
und Quasiimpuls  $\hbar\vec{K}$



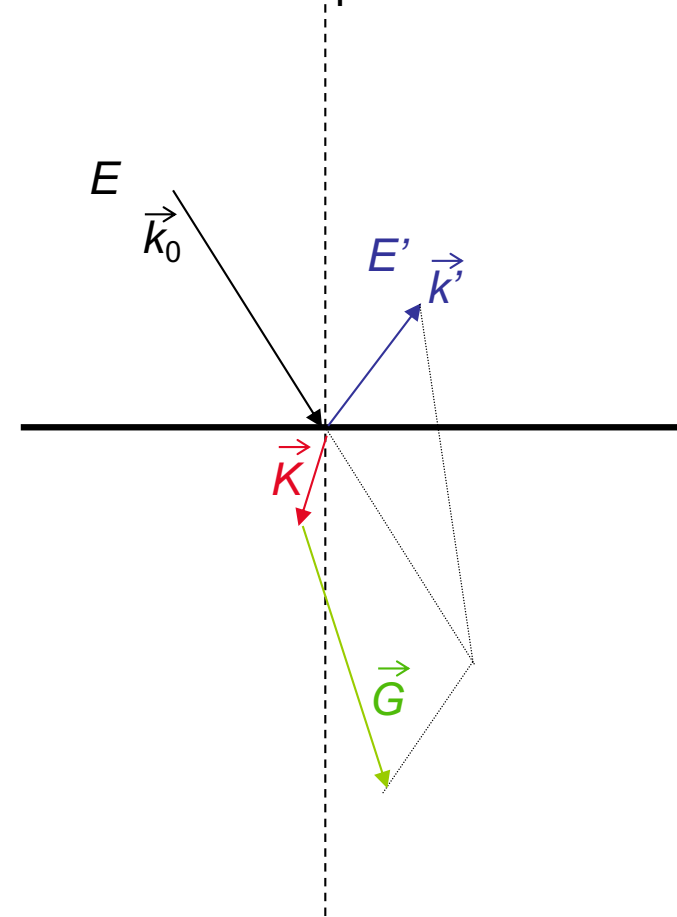
Der Quasiimpuls ist nicht eindeutig: bei gegebenen  $\vec{k}_0, \vec{k}'$  gibt es mehrere Streumöglichkeiten!

$$\vec{k}_0 - \vec{k}' = \vec{K} + \vec{G}$$

$$|E - E'| = \hbar\omega(\vec{K})$$

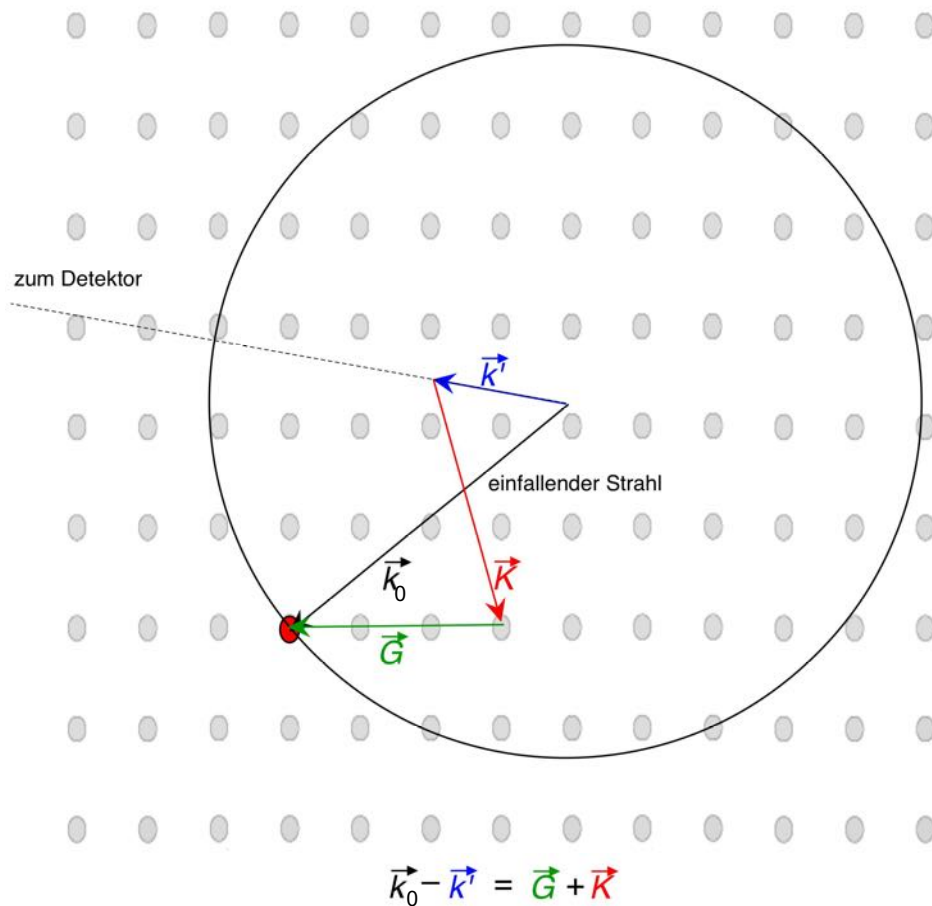


Inelastische Streuung:  
Erzeugung eines Phonons  
mit Energie  $\hbar\omega(\vec{K})$   
und Quasiimpuls  $\hbar\vec{K}$

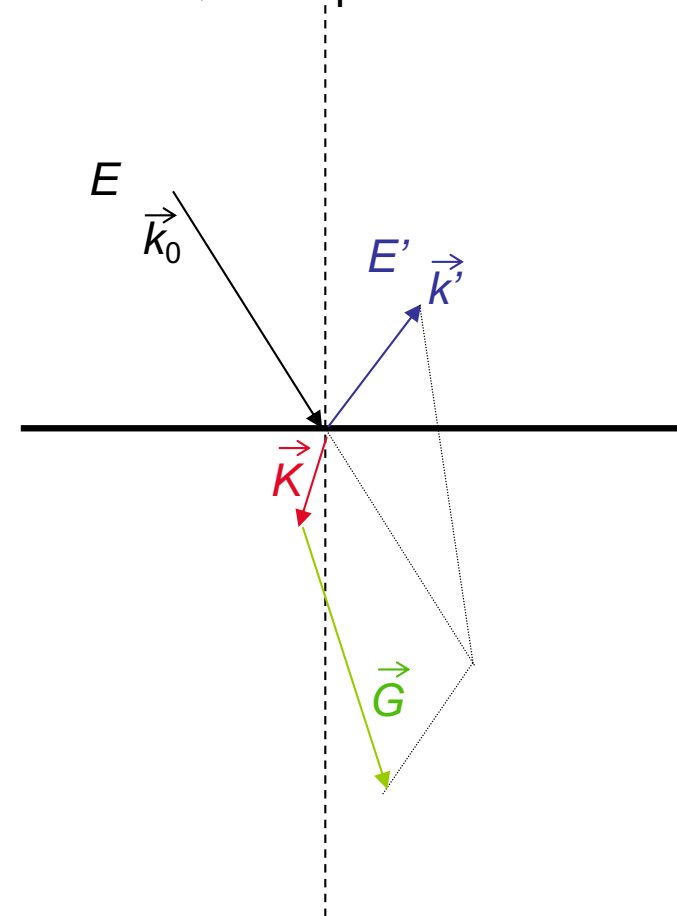


Der Quasiimpuls ist nicht eindeutig: bei gegebenen  $\vec{k}_0, \vec{k}'$  gibt es mehrere Streumöglichkeiten!

$$\begin{aligned} \vec{k}_0 - \vec{k}' &= \vec{K} + \vec{G} \\ |E - E'| &= \hbar\omega(\vec{K}) \end{aligned}$$



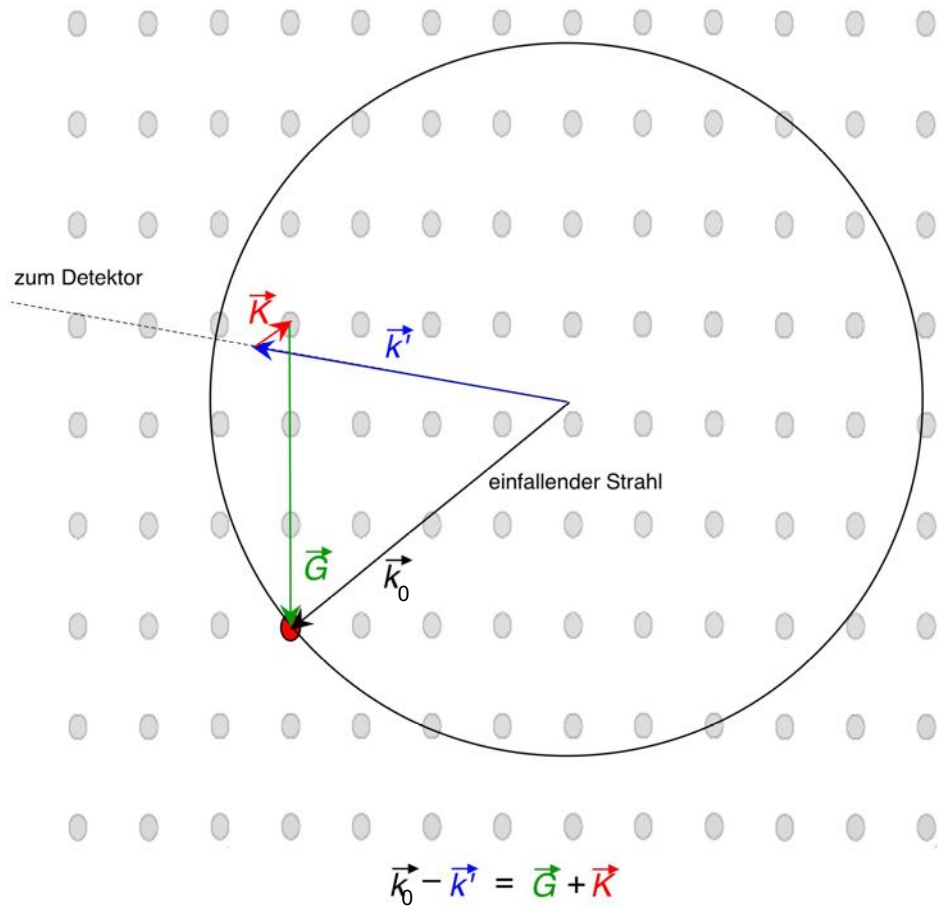
Inelastische Streuung:  
Erzeugung eines Phonons  
mit Energie  $\hbar\omega(\vec{K})$   
und Quasiimpuls  $\hbar\vec{K}$



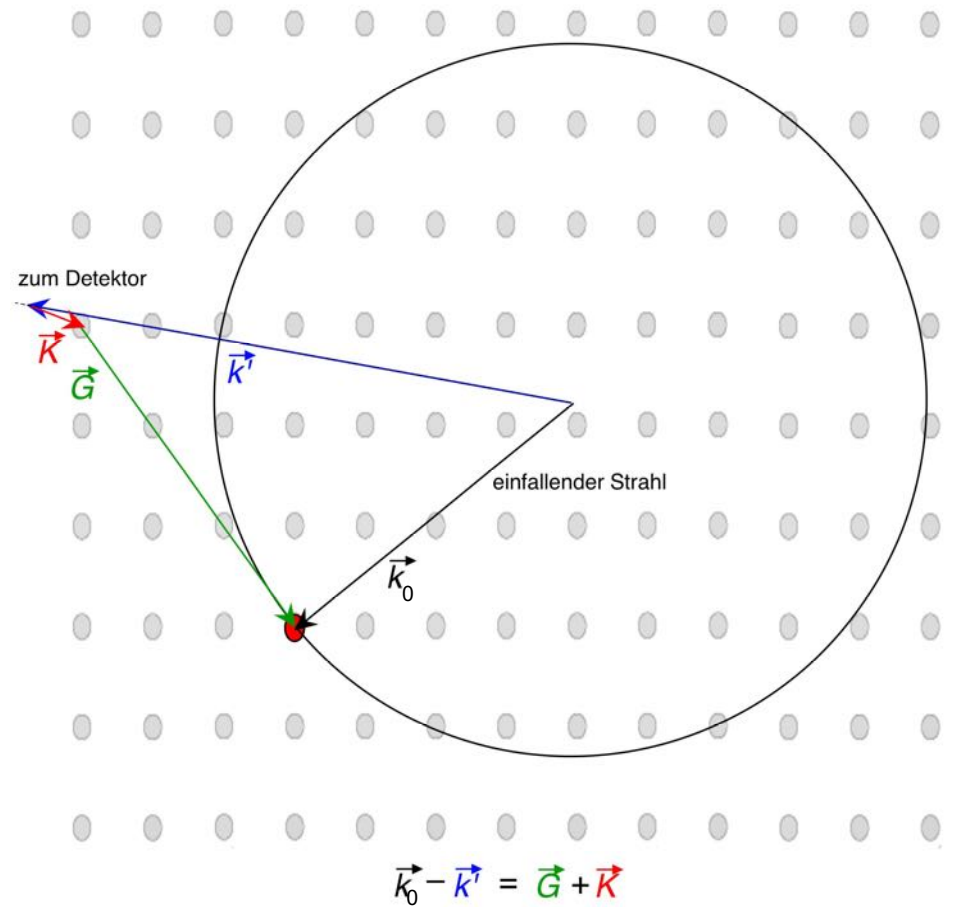
Der Quasiimpuls ist nicht eindeutig: bei gegebenen  $\vec{k}_0, \vec{k}'$  gibt es mehrere Streumöglichkeiten!

$$\vec{k}_0 - \vec{k}' = \vec{K} + \vec{G}$$

$$|E - E'| = \hbar\omega(\vec{K})$$



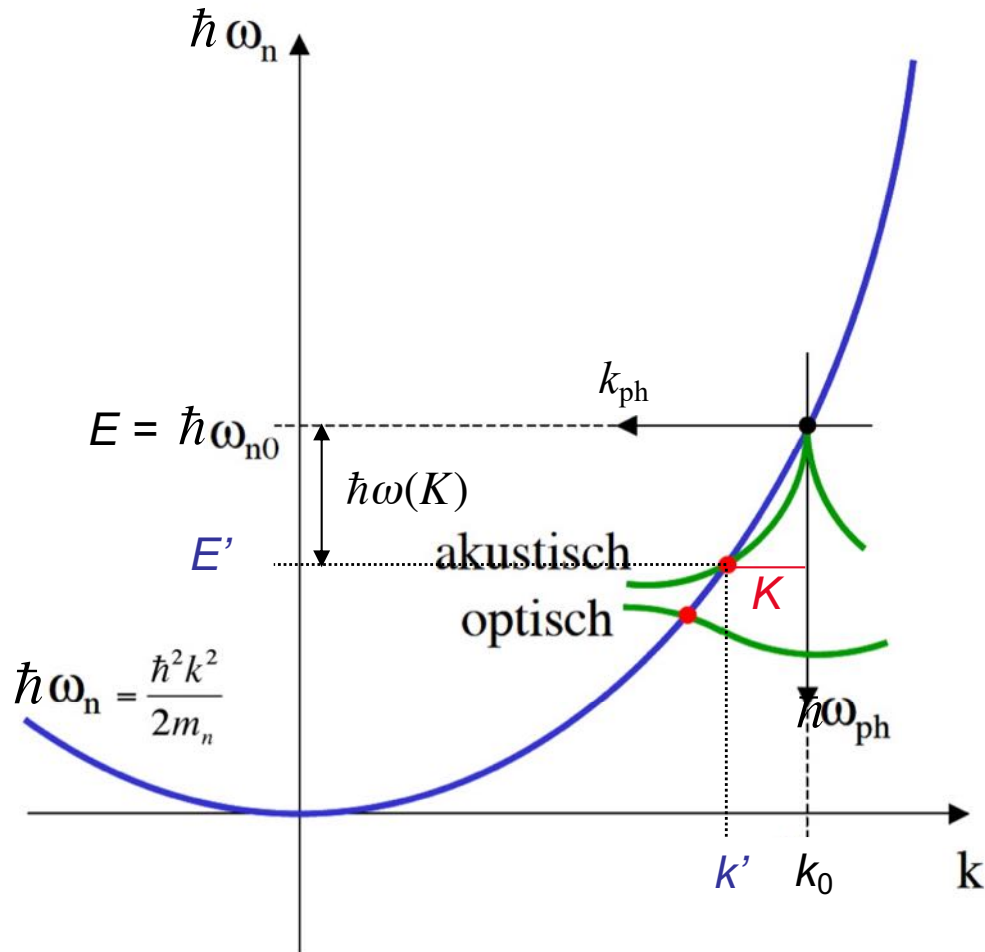
$E - E' > 0$ :  $\vec{k}'$  innerhalb der Ewald-Kugel  
**= Phononen-Erzeugung**



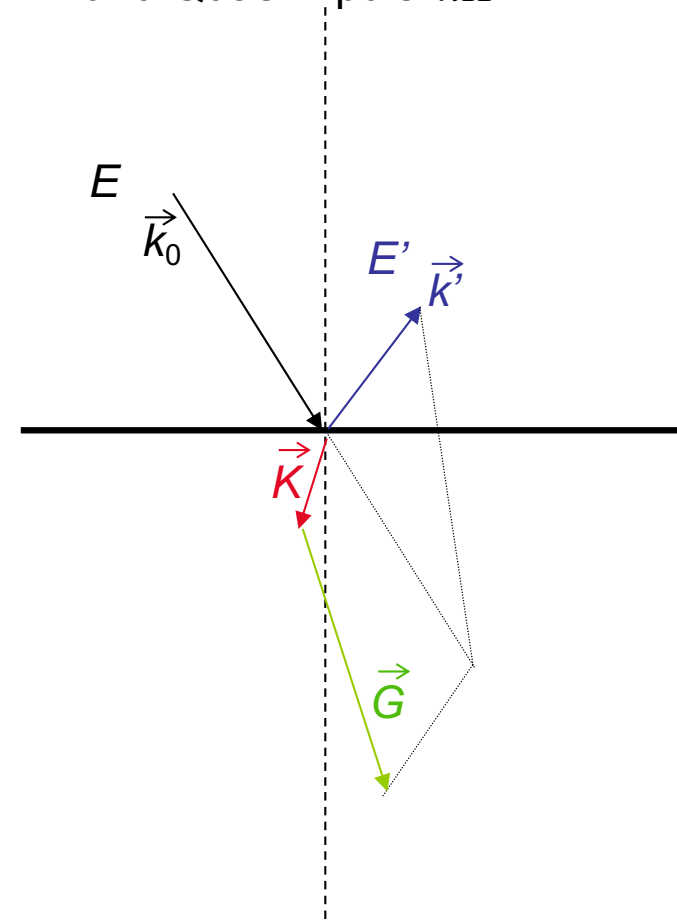
$E - E' < 0$ :  $\vec{k}'$  ausserhalb der Ewald-Kugel  
**= Phononen-Vernichtung**



Phononen-Erzeugung durch Neutronen  
(1D-Veranschaulichung)



Inelastische Streuung:  
Erzeugung eines Phonons  
mit Energie  $\hbar\omega(\vec{K})$   
und Quasiimpuls  $\hbar\vec{K}$

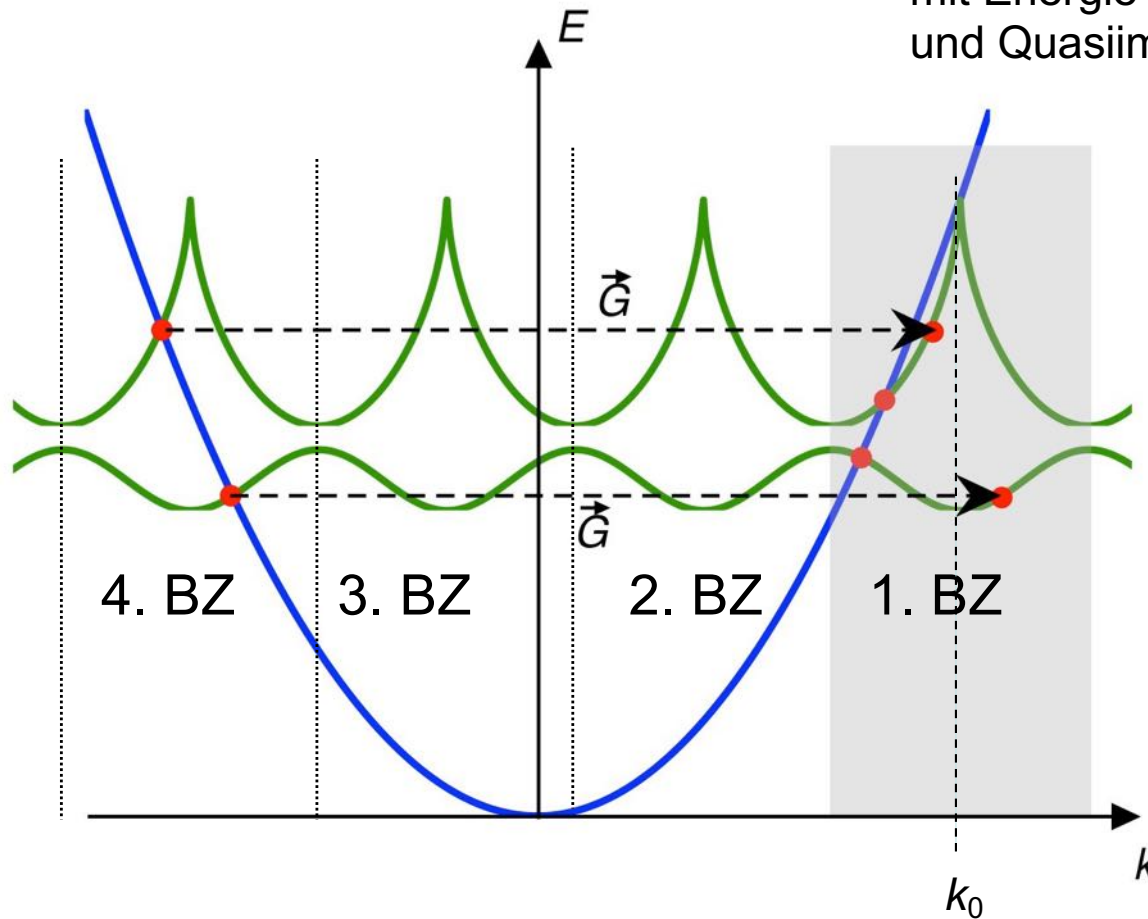


$$\vec{k}_0 - \vec{k}' = \vec{K} + \vec{G}$$

$$|E - E'| = \hbar\omega(\vec{K})$$

Phononen-Erzeugung durch Neutronen  
(1D-Veranschaulichung)

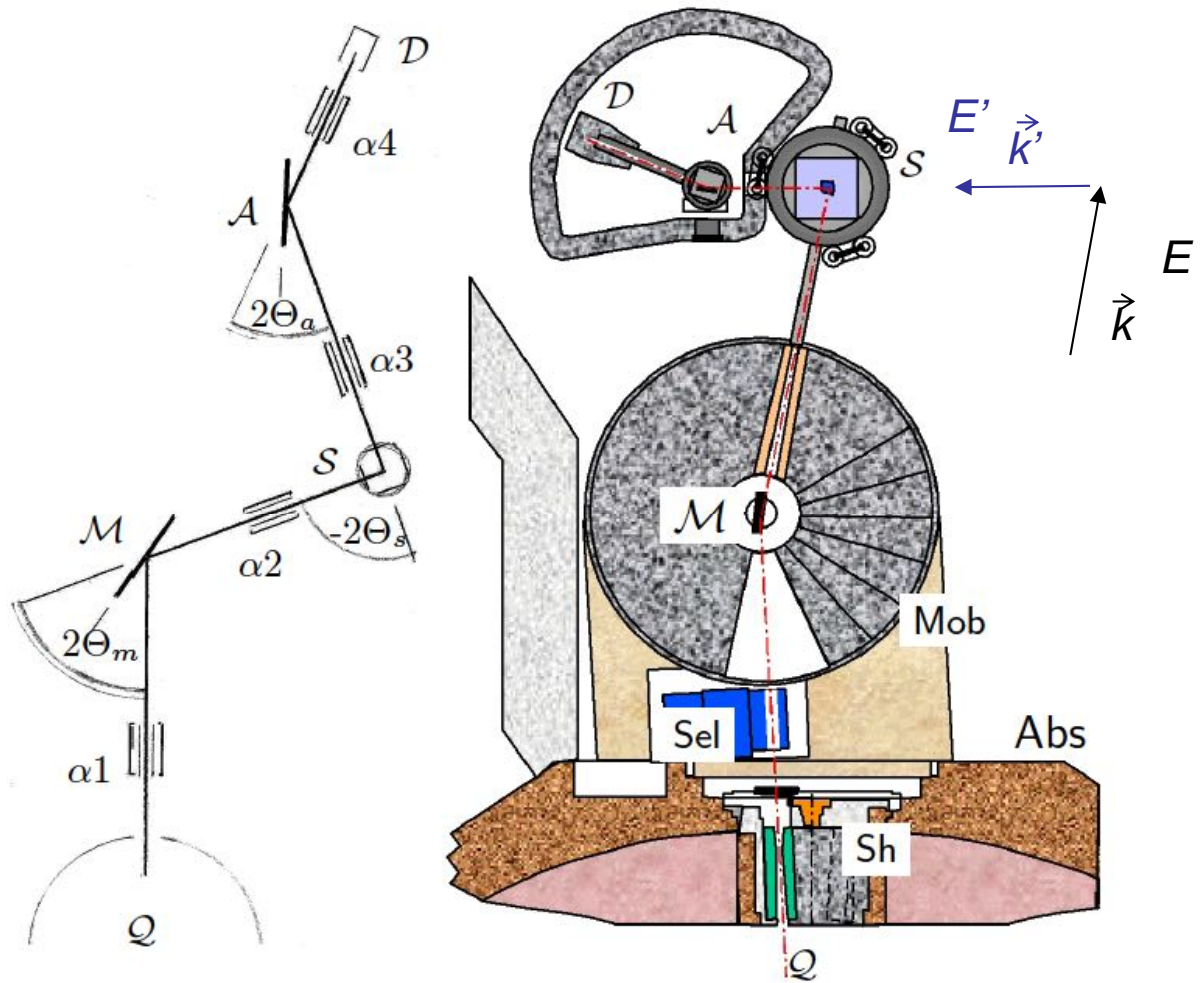
Inelastische Streuung:  
Erzeugung eines Phonons  
mit Energie  $\hbar\omega(\vec{K})$   
und Quasiimpuls  $\hbar\vec{K}$



$$\vec{k}_0 - \vec{k}' = \vec{K} + \vec{G}$$

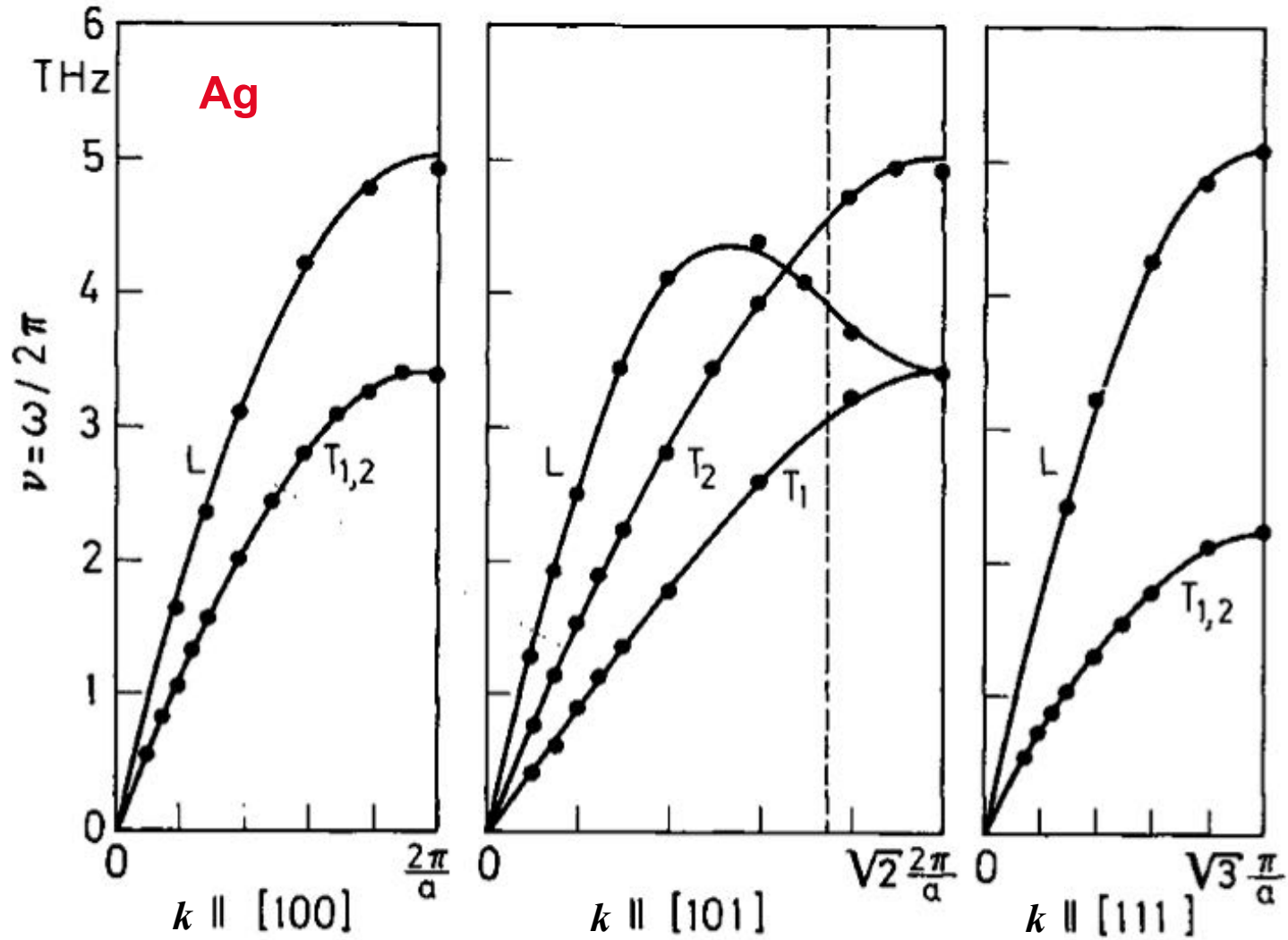
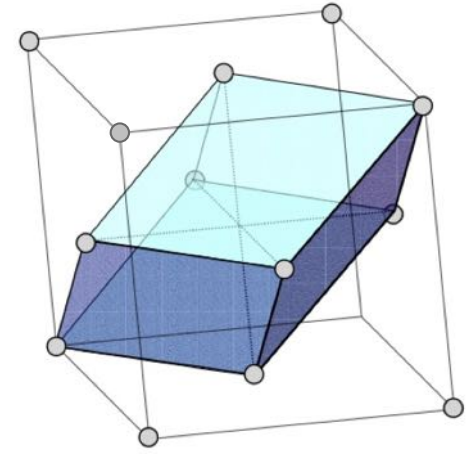
$$|E - E'| = \hbar\omega(\vec{K})$$

$Q$	Neutronenquelle
$M$	Monochromator
$S$	Probentisch
$A$	Analysator
$D$	Detektor
$\alpha_1$ $\alpha_2$ $\alpha_3$ $\alpha_4$	Kollimatoren
$2\theta_m$ $2\theta_s$ $2\theta_a$	Winkel der Spektrometer- achsen
Abs Sel Mob Sh	Abschirmburg Selektor Mobilblöcke Primärshutter

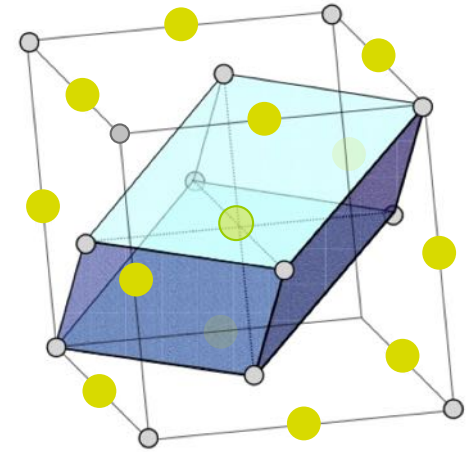
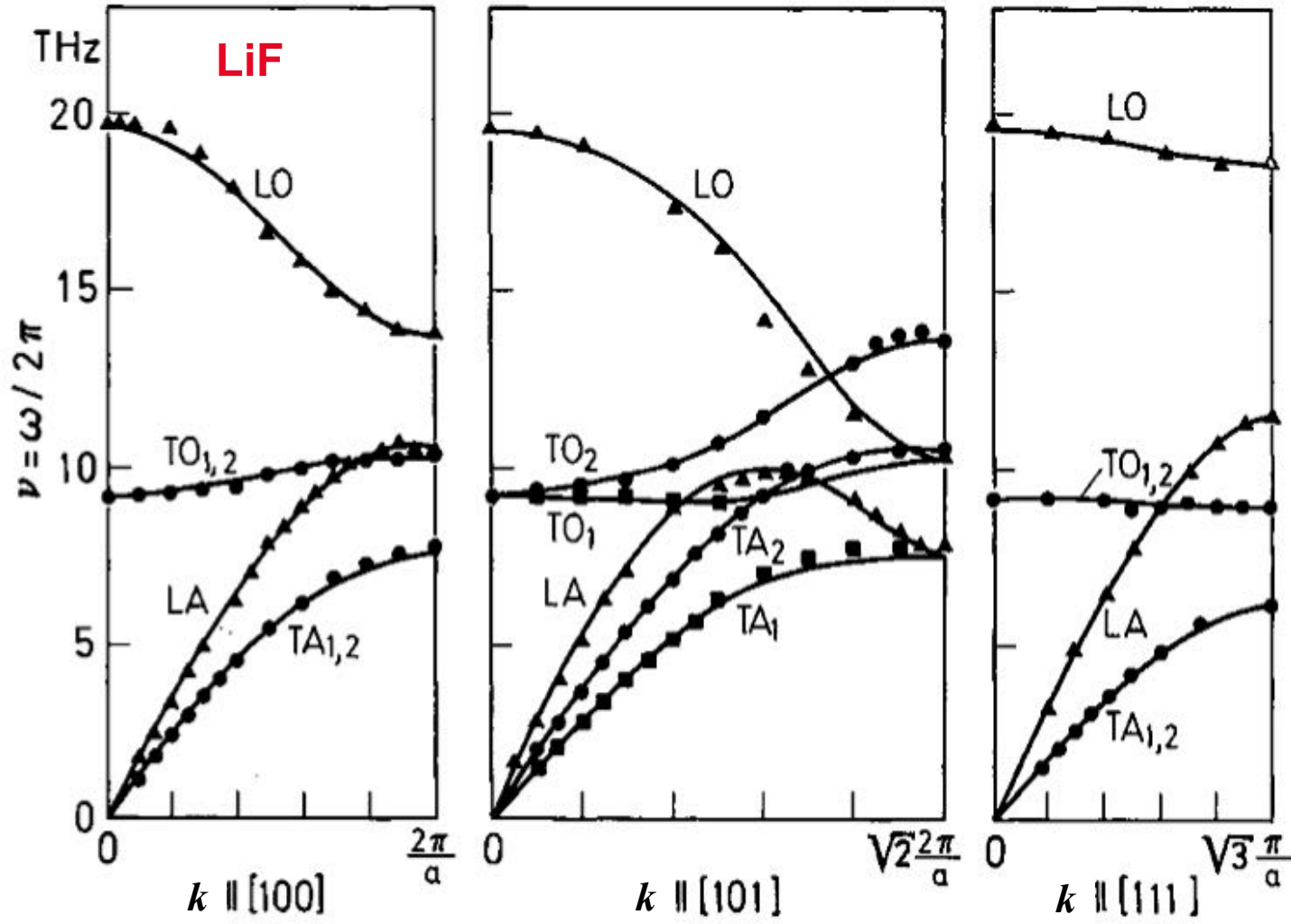


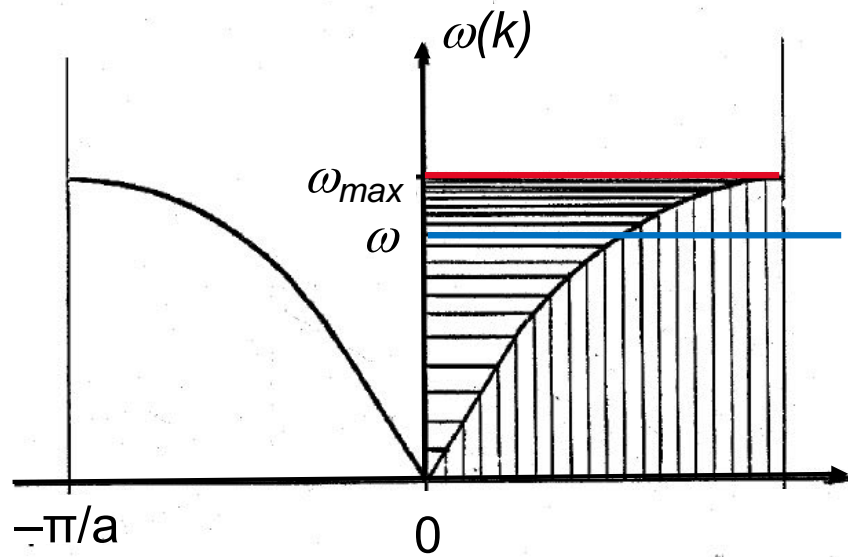
*Schematischer Aufbau eines Dreiachsenspektrometers.*

# 1-atomige Basis



# 2-atomige Basis



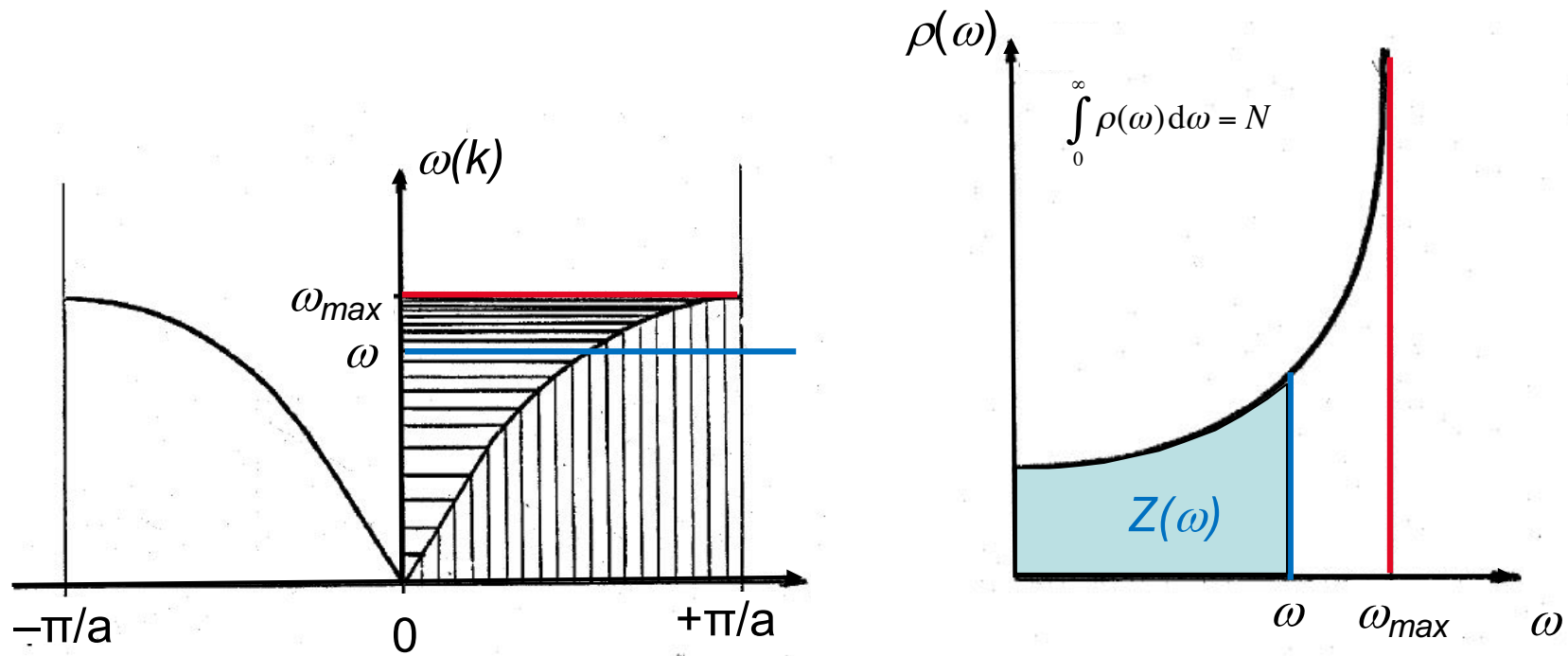


Zustandsdichte  $\rho(\omega) = dZ/d\omega$ :

Anzahl Eigenschwingungen pro Frequenzintervall  $d\omega$

lineare Federkette mit 1-atomiger Basis

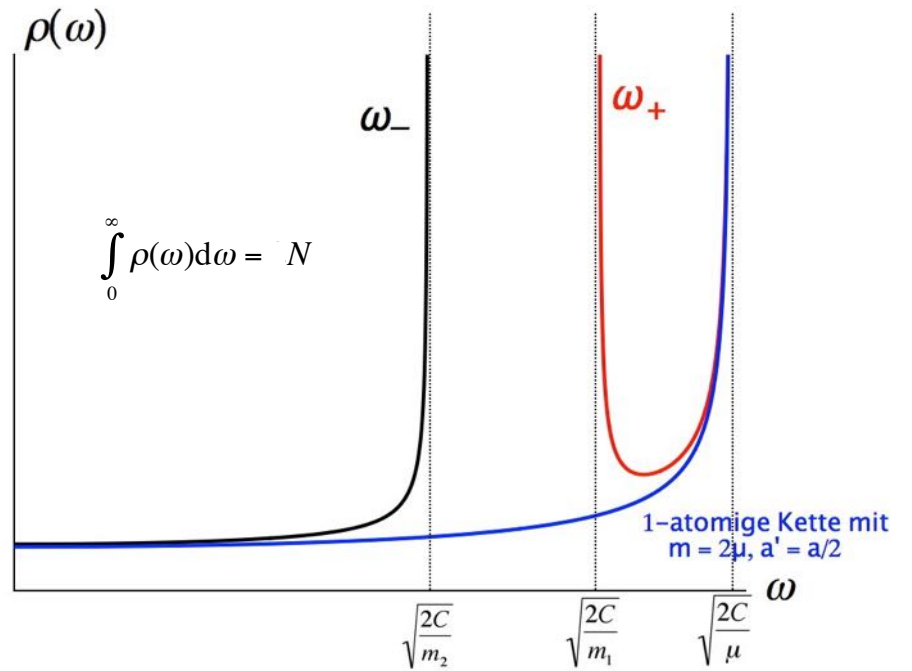
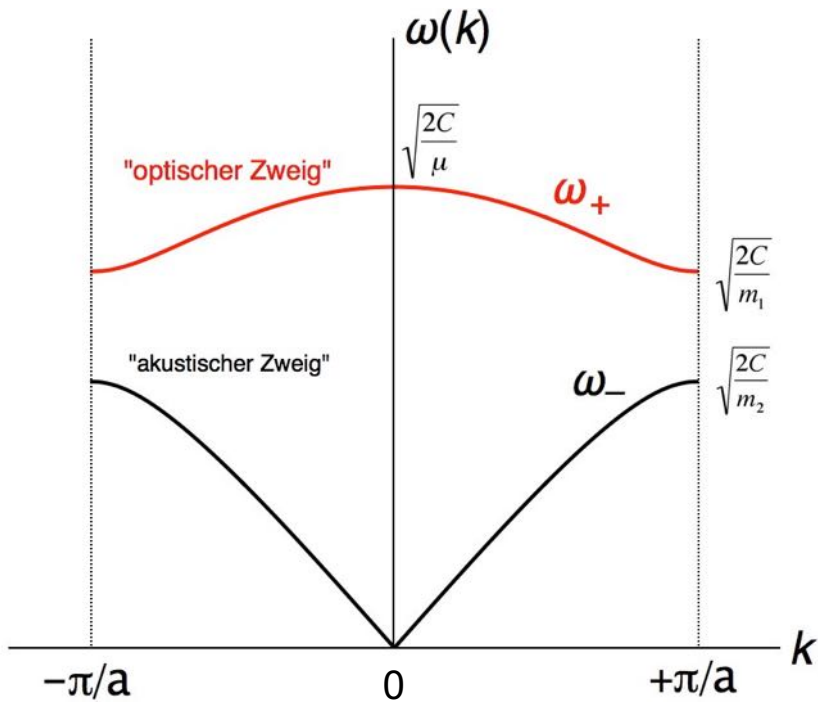
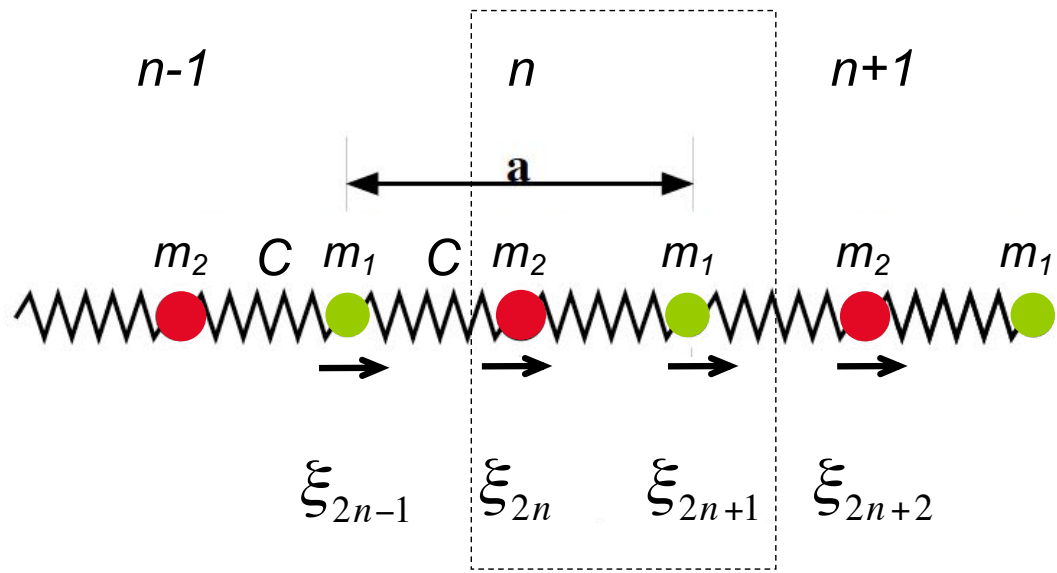




Zustandsdichte  $\rho(\omega) = dZ/d\omega$ :

Anzahl Eigenschwingungen pro Frequenzintervall  $d\omega$

lineare Federkette mit 1-atomiger Basis



lineare Federkette mit 2-atomiger Basis